



Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 +) -1.34
logP (neutral XH) 3.04
logP (X -) -1.62

18C-01008 Points 1 to 32

M16_octanol concentration factor 0.795
Carbonate 0.0308 mM
Acidity error 3.10957 mM

18C-01008 Points 33 to 60

M16_octanol concentration factor 0.841
Carbonate 0.2347 mM
Acidity error 2.72359 mM

18C-01008 Points 61 to 95

M16_octanol concentration factor 0.890
Carbonate 0.3111 mM
Acidity error 2.55032 mM

Warnings and errors

Errors None
Warnings User stopped refinement before final result convergence occurred

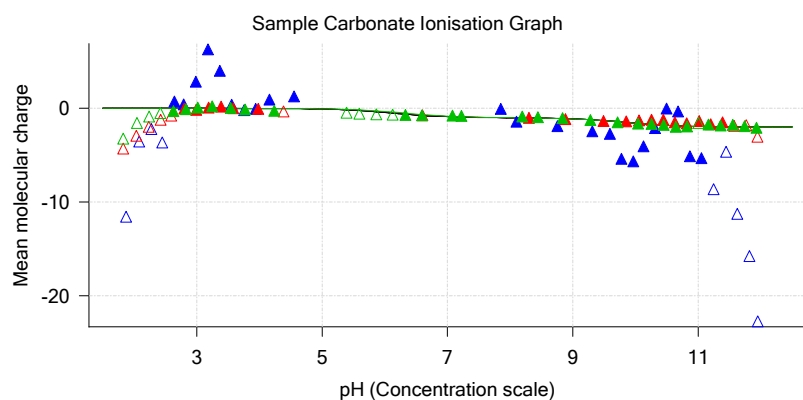
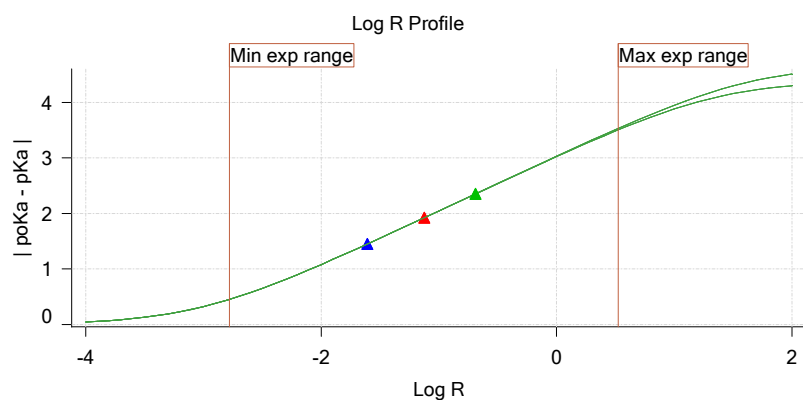
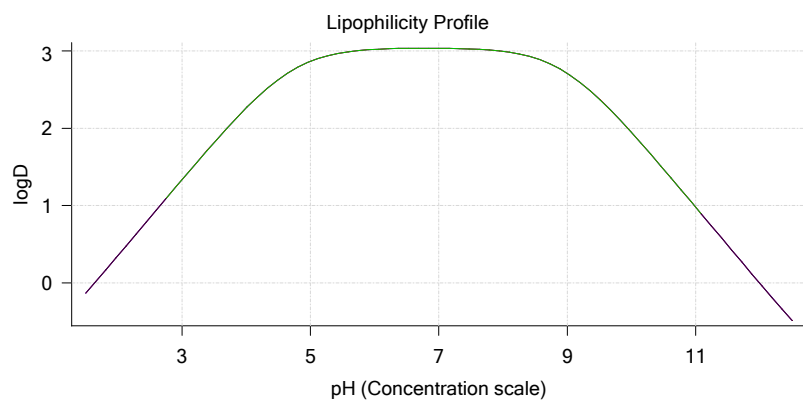
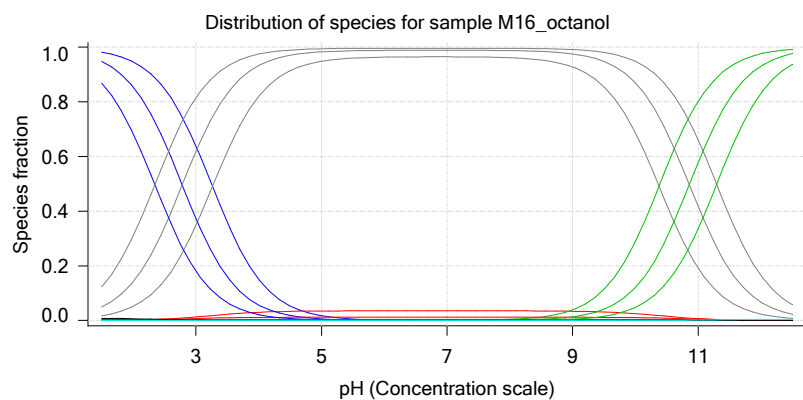
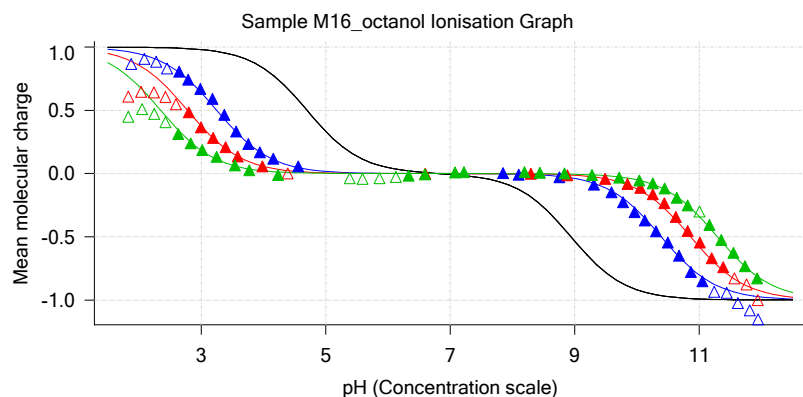
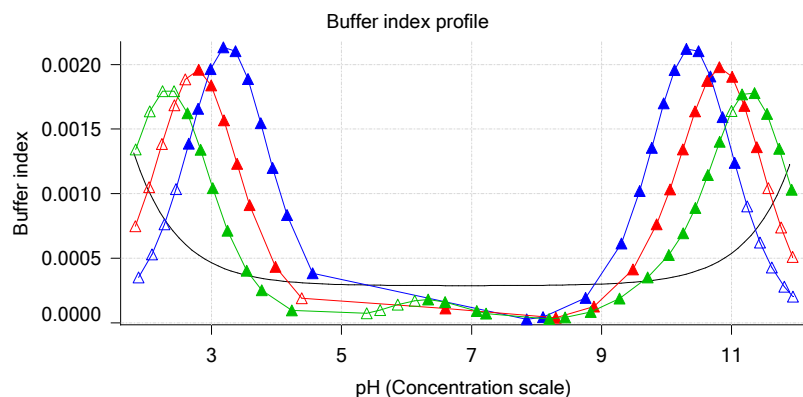
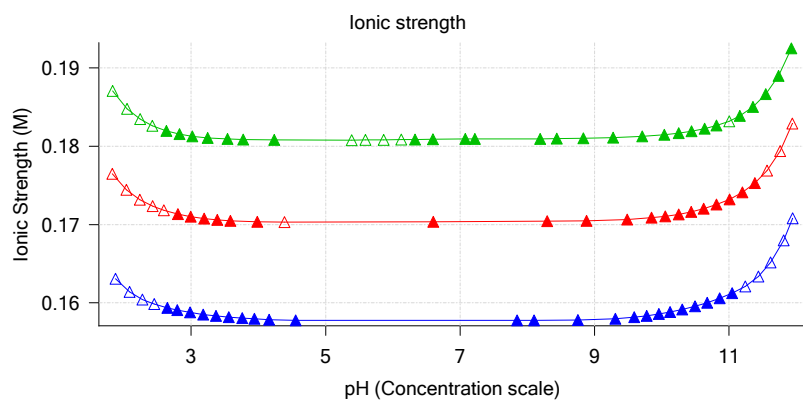
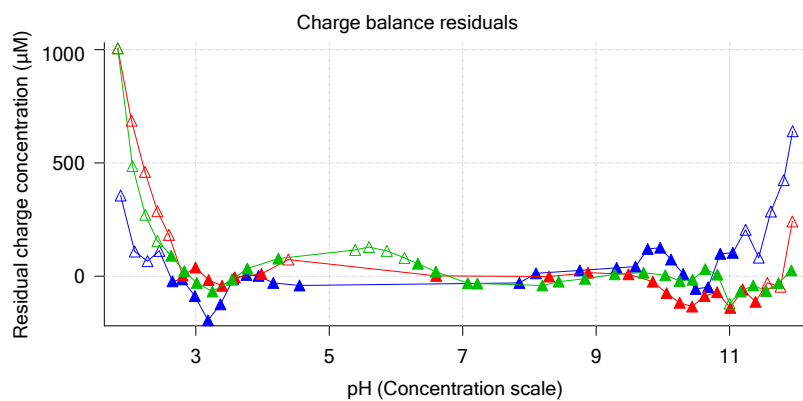
Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.58	79.04 %	0.02 %	0.00 %	3.57 %	17.37 %	0.00 %	Stomach pH
1.200	-0.41	71.75 %	0.02 %	0.00 %	3.24 %	24.99 %	0.00 %	
2.000	0.35	30.82 %	0.06 %	0.00 %	1.39 %	67.73 %	0.00 %	
3.000	1.33	4.34 %	0.09 %	0.00 %	0.20 %	95.38 %	0.00 %	Blood pH
4.000	2.26	0.45 %	0.09 %	0.00 %	0.02 %	99.44 %	0.00 %	
5.000	2.87	0.05 %	0.09 %	0.00 %	0.00 %	99.86 %	0.00 %	
6.000	3.02	0.00 %	0.09 %	0.00 %	0.00 %	99.90 %	0.00 %	
6.500	3.03	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	
7.000	3.03	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	
7.400	3.03	0.00 %	0.09 %	0.00 %	0.00 %	99.91 %	0.00 %	
8.000	2.99	0.00 %	0.09 %	0.01 %	0.00 %	99.90 %	0.00 %	
9.000	2.71	0.00 %	0.09 %	0.10 %	0.00 %	99.80 %	0.00 %	
10.000	1.95	0.00 %	0.09 %	1.03 %	0.00 %	98.85 %	0.02 %	
11.000	0.98	0.00 %	0.08 %	9.41 %	0.00 %	90.28 %	0.23 %	
12.000	-0.01	0.00 %	0.04 %	50.40 %	0.00 %	48.35 %	1.21 %	

Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

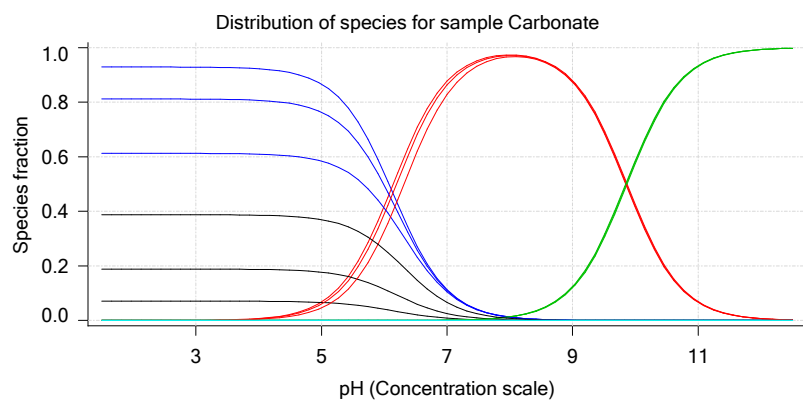
Graphs



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Graphs (continued)



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-01008 Points 1 to 32

Overall results

RMSD 0.203
 Average ionic strength 0.159 M
 Average temperature 25.0°C
 Partition ratio 0.0247 : 1
 Analyte concentration range 4379.7 µM to 4702.9 µM
 Total points considered 23 of 32

Warnings and errors

Errors None
 Warnings Excessive acidity error present

Four-Plus parameters

Alpha 0.130 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r

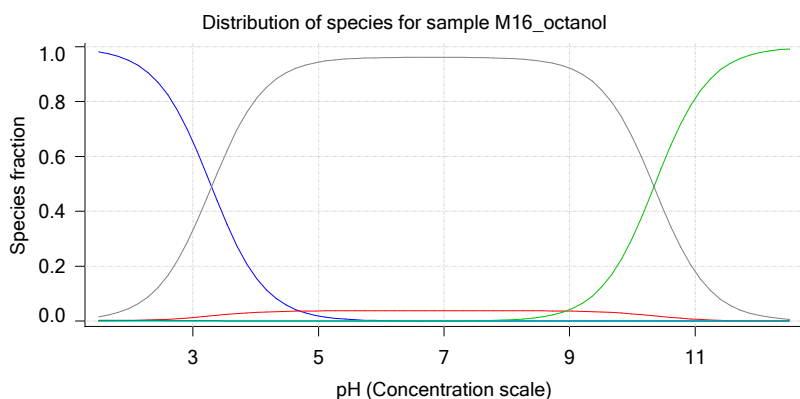
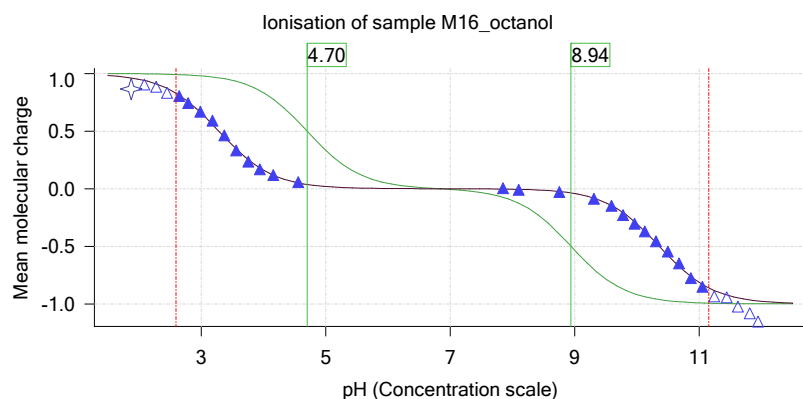
Titants

0.50 M HCl 0.993513 3/1/2018 10:41:05 AM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 10:41:05 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor 0.795
 Base pKa 1 4.70
 Acid pKa 2 8.94
 logP (XH₂⁺) -0.95
 logP (neutral XH) 3.01
 logP (X⁻) -1.62

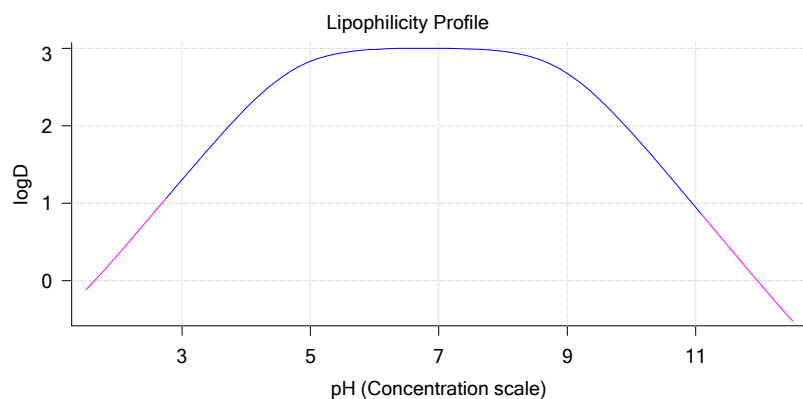
Sample graphs



Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



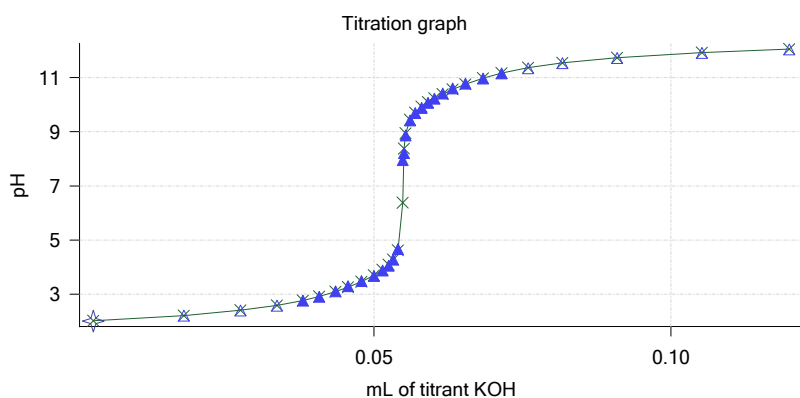
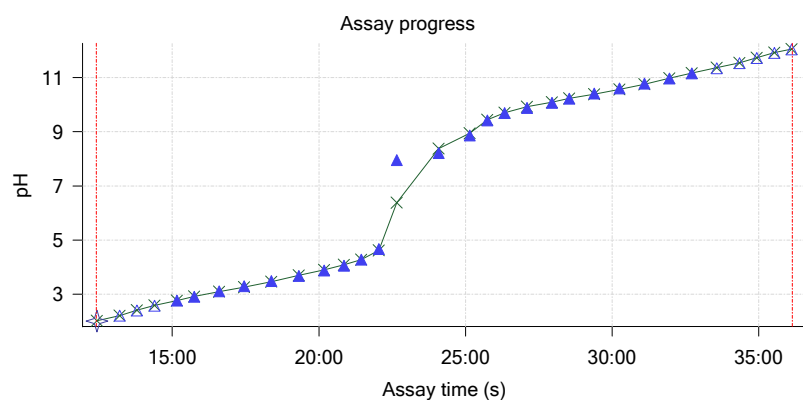
Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.50	99.20 %	0.02 %	0.00 %	0.28 %	0.50 %	0.00 %	Stomach pH
1.200	-0.36	98.90 %	0.03 %	0.00 %	0.27 %	0.79 %	0.00 %	
2.000	0.33	94.77 %	0.19 %	0.00 %	0.26 %	4.78 %	0.00 %	
3.000	1.30	65.49 %	1.31 %	0.00 %	0.18 %	33.02 %	0.00 %	
4.000	2.23	16.01 %	3.19 %	0.00 %	0.04 %	80.75 %	0.00 %	
5.000	2.83	1.87 %	3.73 %	0.00 %	0.01 %	94.39 %	0.00 %	
6.000	2.99	0.19 %	3.80 %	0.00 %	0.00 %	96.01 %	0.00 %	Blood pH
6.500	3.00	0.06 %	3.80 %	0.01 %	0.00 %	96.12 %	0.00 %	
7.000	3.00	0.02 %	3.80 %	0.04 %	0.00 %	96.13 %	0.00 %	
7.400	3.00	0.01 %	3.80 %	0.11 %	0.00 %	96.08 %	0.00 %	
8.000	2.96	0.00 %	3.79 %	0.44 %	0.00 %	95.77 %	0.00 %	
9.000	2.68	0.00 %	3.65 %	4.19 %	0.00 %	92.16 %	0.00 %	
10.000	1.91	0.00 %	2.65 %	30.40 %	0.00 %	66.93 %	0.02 %	
11.000	0.95	0.00 %	0.71 %	81.34 %	0.00 %	17.91 %	0.05 %	
12.000	-0.04	0.00 %	0.09 %	97.71 %	0.00 %	2.15 %	0.06 %	

Carbonate and acidity

Carbonate 0.031 mM
Acidity error 3.110 mM

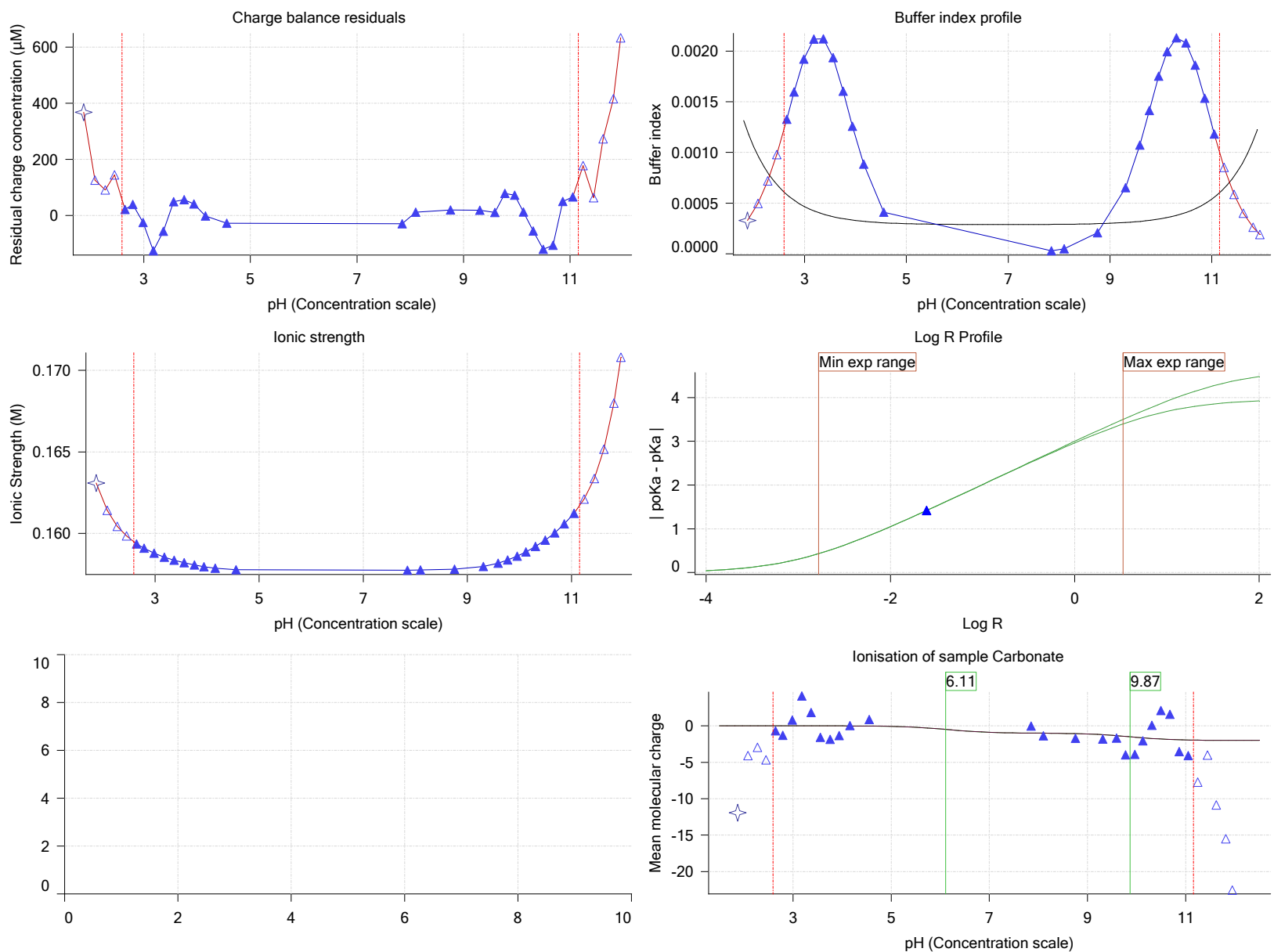
Other graphs



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-01008 Points 33 to 60

Overall results

RMSD 0.036
 Average ionic strength 0.171 M
 Average temperature 25.0°C
 Partition ratio 0.0751 : 1
 Analyte concentration range 3612.7 µM to 3864.7 µM
 Total points considered 19 of 28

Warnings and errors

Errors None
 Warnings Excessive acidity error present

Four-Plus parameters

Alpha 0.130 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r

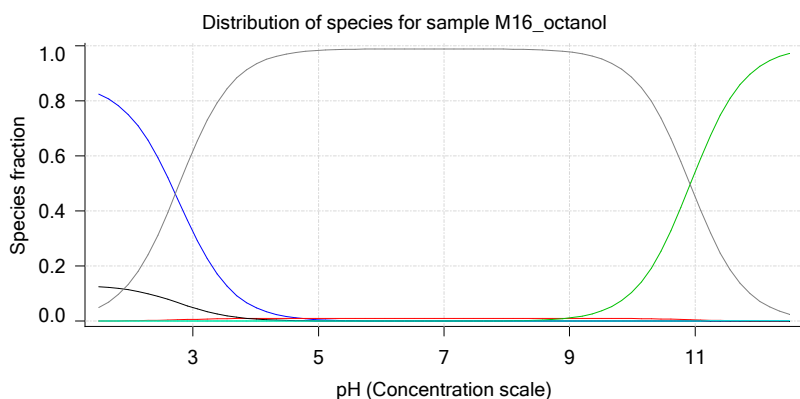
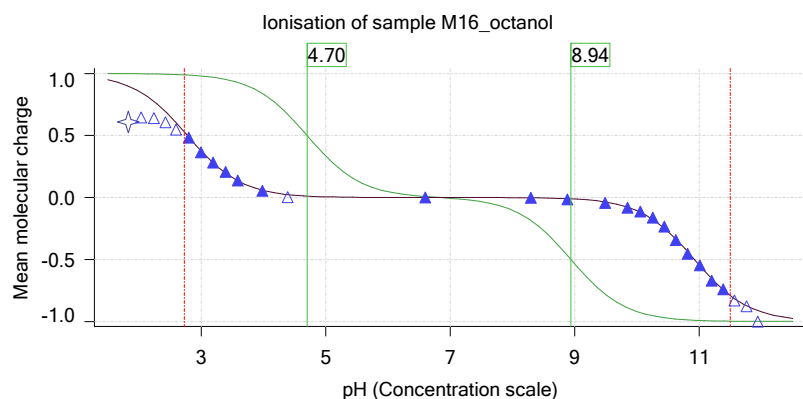
Titrants

0.50 M HCl 0.993513 3/1/2018 10:41:05 AM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 10:41:05 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor 0.841
 Base pKa 1 4.70
 Acid pKa 2 8.94
 logP (XH₂⁺) 0.31
 logP (neutral XH) 3.10
 logP (X⁻) -1.62

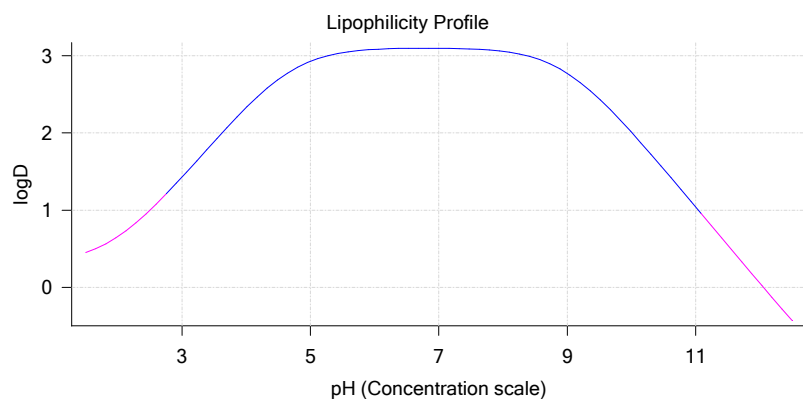
Sample graphs



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



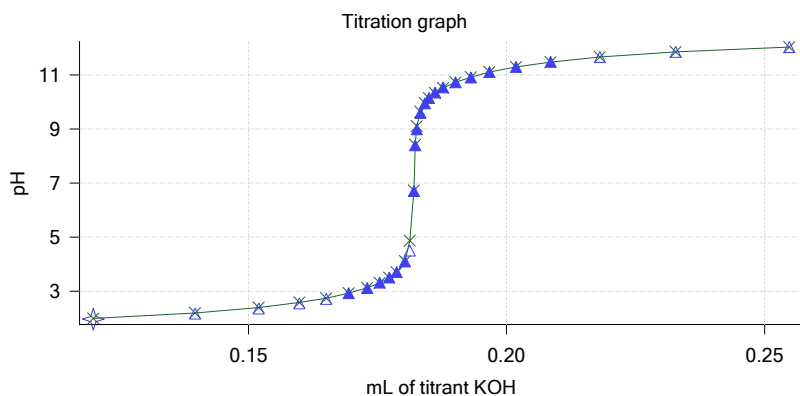
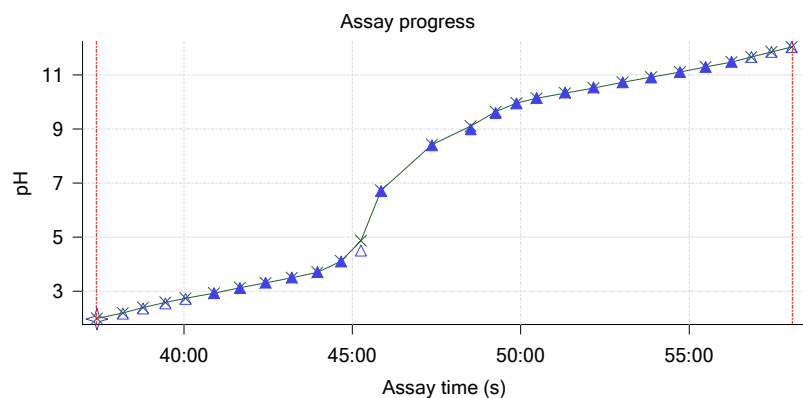
Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	0.36	85.40 %	0.02 %	0.00 %	12.96 %	1.62 %	0.00 %	Stomach pH
1.200	0.38	84.59 %	0.03 %	0.00 %	12.83 %	2.55 %	0.00 %	
2.000	0.66	74.43 %	0.15 %	0.00 %	11.29 %	14.13 %	0.00 %	
3.000	1.43	32.57 %	0.65 %	0.00 %	4.94 %	61.84 %	0.00 %	
4.000	2.33	4.92 %	0.98 %	0.00 %	0.75 %	93.36 %	0.00 %	
5.000	2.93	0.52 %	1.03 %	0.00 %	0.08 %	98.37 %	0.00 %	Blood pH
6.000	3.08	0.05 %	1.04 %	0.00 %	0.01 %	98.90 %	0.00 %	
6.500	3.09	0.02 %	1.04 %	0.00 %	0.00 %	98.94 %	0.00 %	
7.000	3.10	0.01 %	1.04 %	0.01 %	0.00 %	98.94 %	0.00 %	
7.400	3.09	0.00 %	1.04 %	0.03 %	0.00 %	98.93 %	0.00 %	
8.000	3.06	0.00 %	1.04 %	0.12 %	0.00 %	98.84 %	0.00 %	
9.000	2.77	0.00 %	1.03 %	1.18 %	0.00 %	97.79 %	0.00 %	
10.000	2.01	0.00 %	0.93 %	10.66 %	0.00 %	88.39 %	0.02 %	
11.000	1.04	0.00 %	0.47 %	54.37 %	0.00 %	45.06 %	0.10 %	
12.000	0.05	0.00 %	0.08 %	92.12 %	0.00 %	7.64 %	0.17 %	

Carbonate and acidity

Carbonate 0.235 mM
 Acidity error 2.724 mM

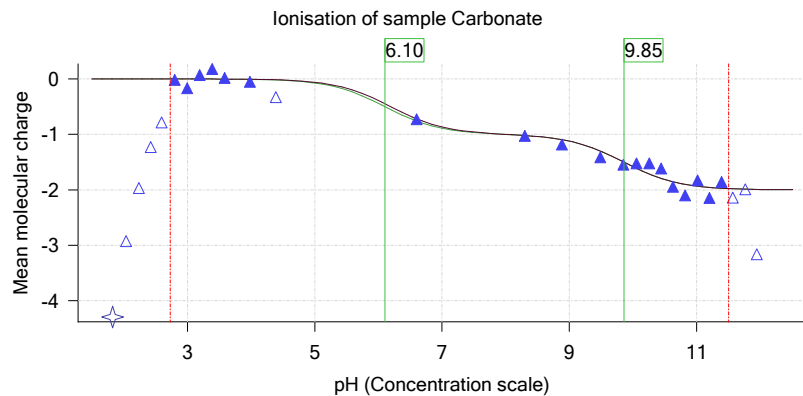
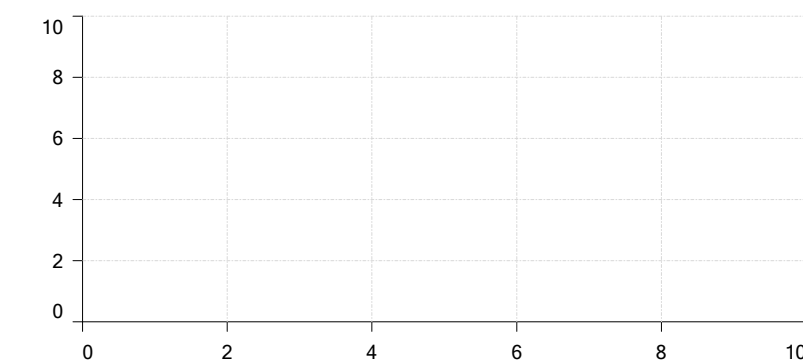
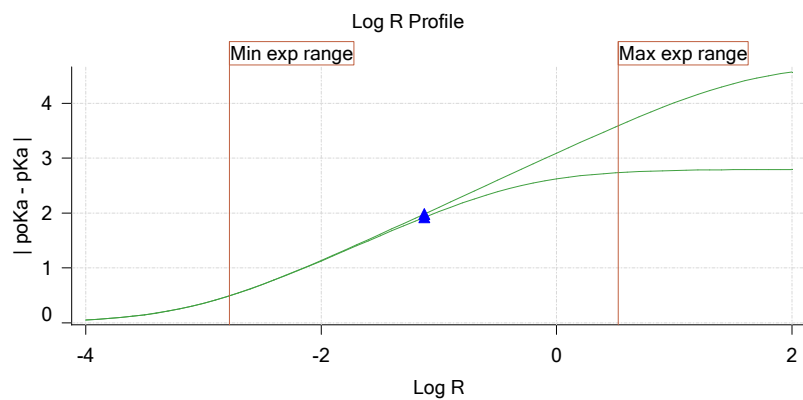
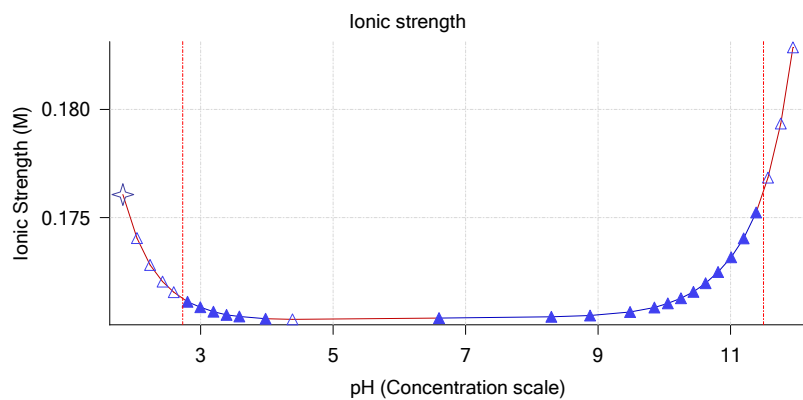
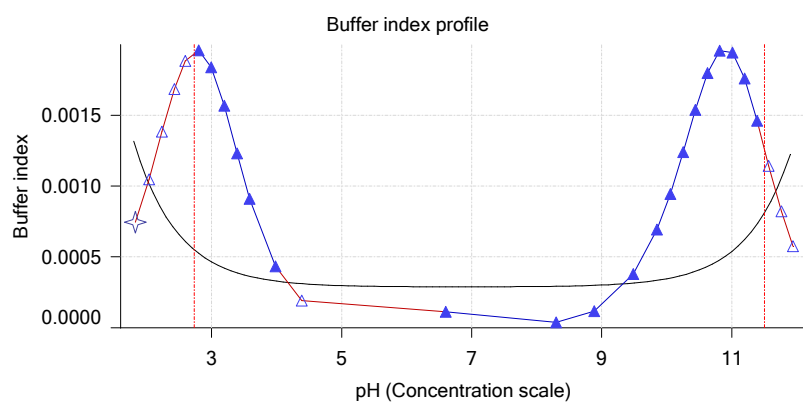
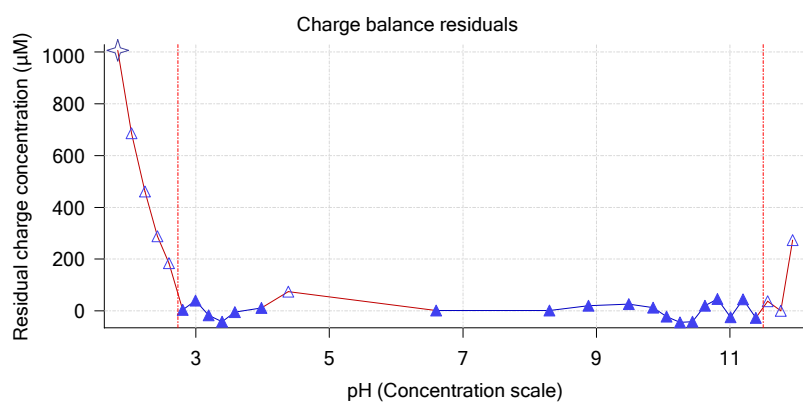
Other graphs



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 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-01008 Points 61 to 95

Overall results

RMSD 0.274
 Average ionic strength 0.182 M
 Average temperature 25.0°C
 Partition ratio 0.2049 : 1
 Analyte concentration range 2812.2 µM to 2977.4 µM
 Total points considered 26 of 35

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.130 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 S 0.9970 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jH 0.8 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r
 jOH -0.4 3/1/2018 10:41:04 AM C:\Sirius_T3\HCl18B27.t3r

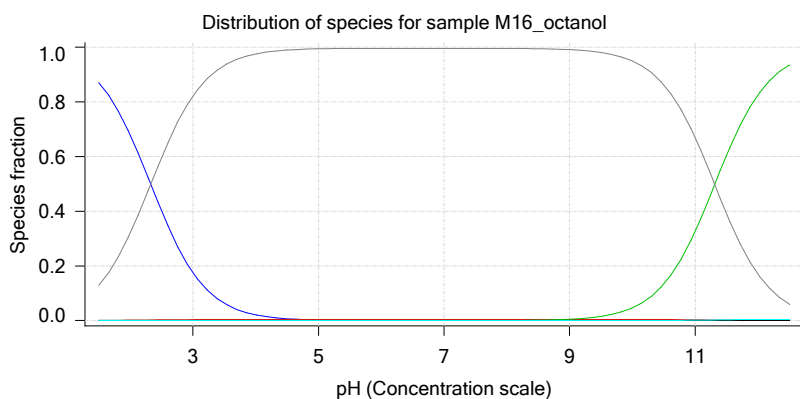
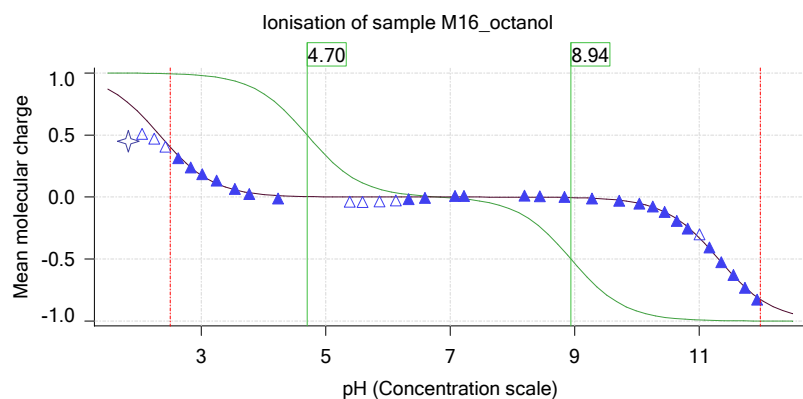
Titrants

0.50 M HCl 0.993513 3/1/2018 10:41:05 AM C:\Sirius_T3\HCl18B27.t3r
 0.50 M KOH 0.999845 3/1/2018 10:41:05 AM C:\Sirius_T3\KOH18B27.t3r

Sample

M16_octanol concentration factor 0.890
 Base pKa 1 4.70
 Acid pKa 2 8.94
 logP (XH₂⁺) -3.82
 logP (neutral XH) 3.06
 logP (X⁻) -1.62

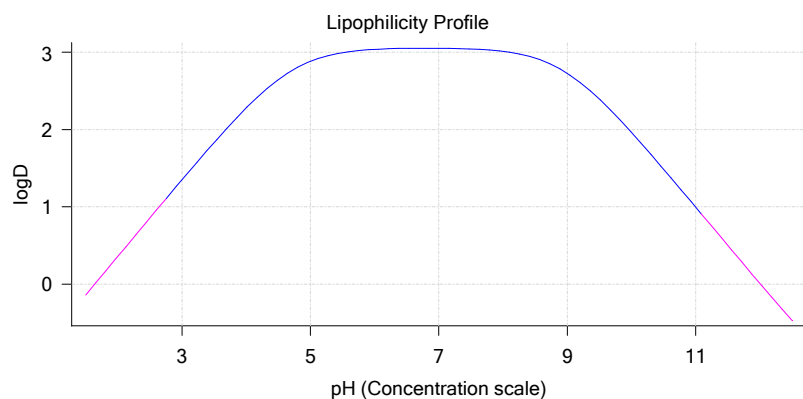
Sample graphs



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



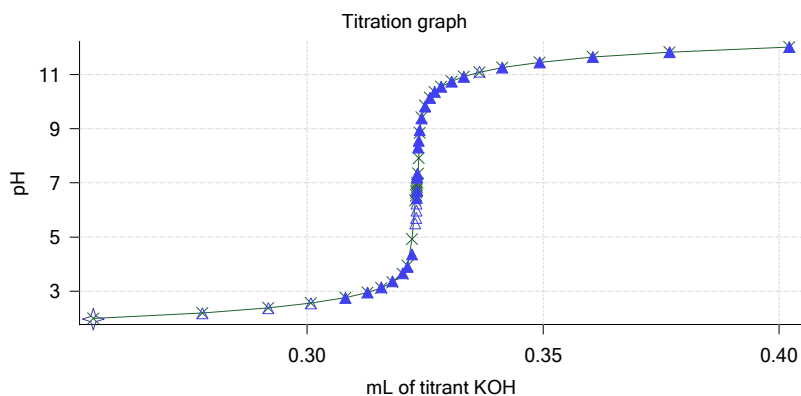
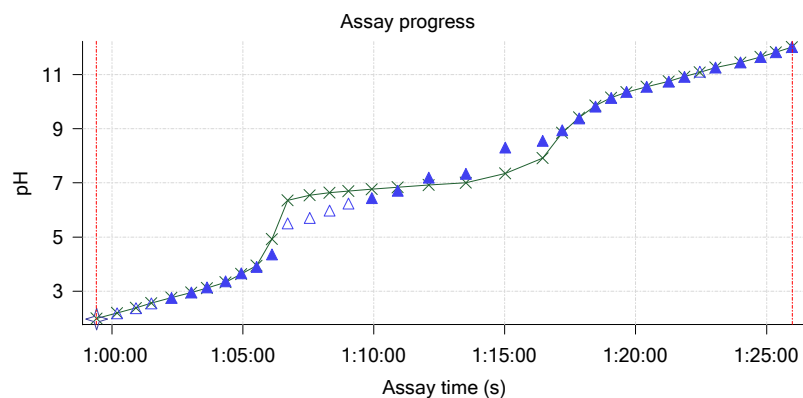
Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.64	95.51 %	0.02 %	0.00 %	0.00 %	4.47 %	0.00 %	Stomach pH
1.200	-0.44	93.06 %	0.03 %	0.00 %	0.00 %	6.91 %	0.00 %	
2.000	0.36	68.01 %	0.14 %	0.00 %	0.00 %	31.85 %	0.00 %	
3.000	1.35	17.53 %	0.35 %	0.00 %	0.00 %	82.12 %	0.00 %	
4.000	2.28	2.08 %	0.42 %	0.00 %	0.00 %	97.50 %	0.00 %	Blood pH
5.000	2.88	0.21 %	0.42 %	0.00 %	0.00 %	99.36 %	0.00 %	
6.000	3.04	0.02 %	0.42 %	0.00 %	0.00 %	99.55 %	0.00 %	
6.500	3.05	0.01 %	0.42 %	0.00 %	0.00 %	99.57 %	0.00 %	
7.000	3.05	0.00 %	0.42 %	0.00 %	0.00 %	99.57 %	0.00 %	
7.400	3.05	0.00 %	0.42 %	0.01 %	0.00 %	99.56 %	0.00 %	
8.000	3.01	0.00 %	0.42 %	0.05 %	0.00 %	99.53 %	0.00 %	
9.000	2.73	0.00 %	0.42 %	0.48 %	0.00 %	99.09 %	0.00 %	
10.000	1.96	0.00 %	0.40 %	4.64 %	0.00 %	94.93 %	0.02 %	
11.000	1.00	0.00 %	0.28 %	32.70 %	0.00 %	66.85 %	0.16 %	
12.000	0.01	0.00 %	0.07 %	82.63 %	0.00 %	16.89 %	0.41 %	

Carbonate and acidity

Carbonate 0.311 mM
 Acidity error 2.550 mM

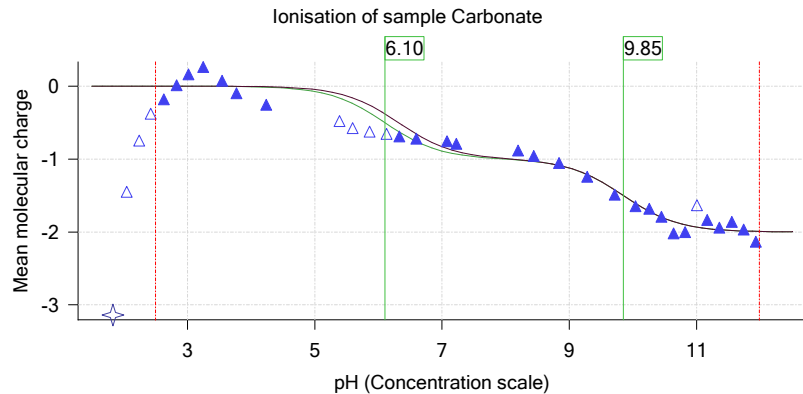
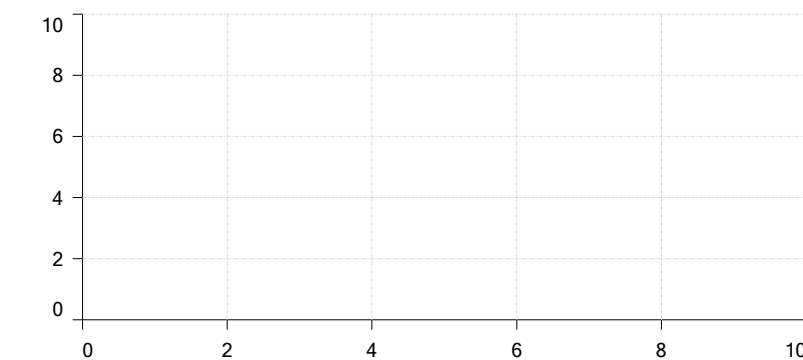
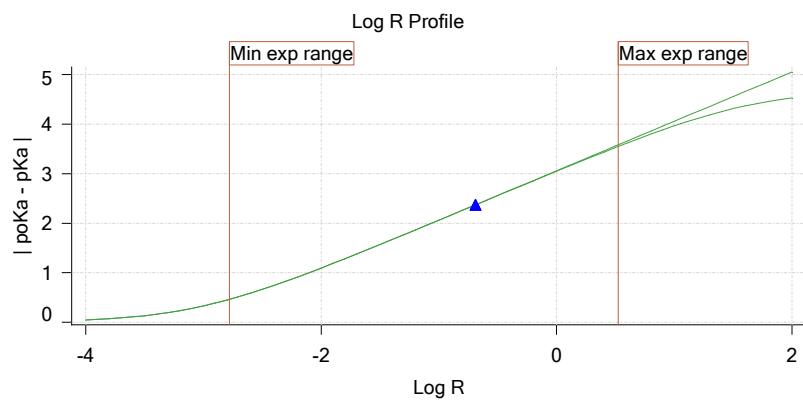
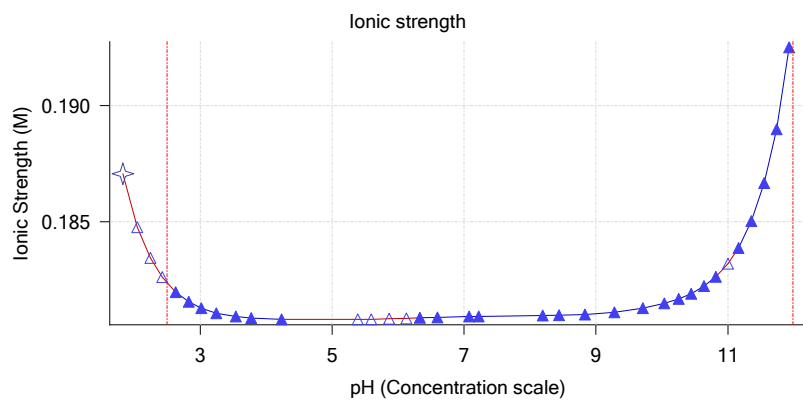
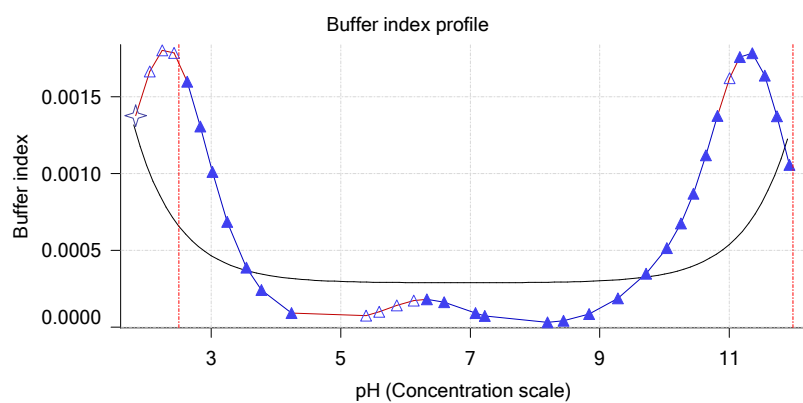
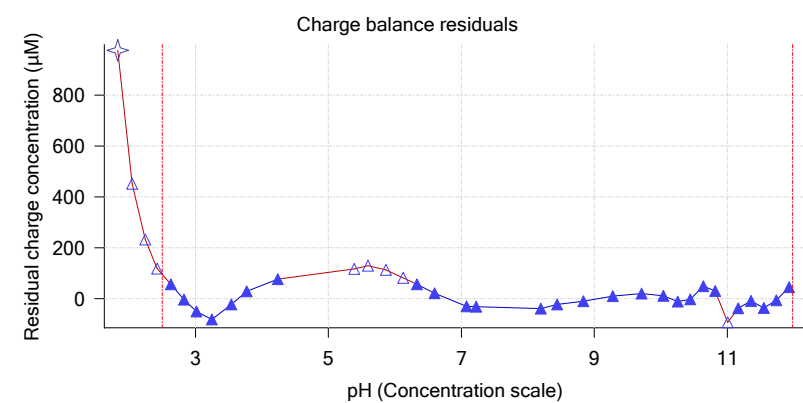
Other graphs



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M16_octanol	2/27/2018 6:14:13 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001570 g	2/28/2018 4:25:47 PM	User entered value
Formula weight	210.23 g/mol	2/27/2018 5:08:55 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	210.23	2/27/2018 5:08:55 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:08:55 PM	User entered value
Sample is a	Ampholyte	2/27/2018 5:08:55 PM	User entered value
pKa 1	4.70	2/27/2018 5:08:55 PM	User entered value
Type	Base	2/27/2018 5:08:55 PM	User entered value
pKa 2	8.94	2/27/2018 5:08:55 PM	User entered value
Type	Acid	2/27/2018 5:08:55 PM	User entered value
logp (XH2 +)	-0.97	2/27/2018 5:09:30 PM	User entered value
logP (neutral XH)	1.47	2/27/2018 5:09:44 PM	User entered value
logP (X -)	-1.62	2/27/2018 5:09:50 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:20.9	Initial pH = 3.61									
12:25.5	Data point 1	1.50000 mL	0.04518 mL	0.00275 mL	0.04000 mL	2.007	-0.00290	0.67446	0.00017	10.5 s
13:12.3	Data point 2	1.50000 mL	0.04518 mL	0.01799 mL	0.04000 mL	2.212	0.00158	0.11489	0.00023	10.0 s
13:47.9	Data point 3	1.50000 mL	0.04518 mL	0.02752 mL	0.04000 mL	2.403	0.00139	0.25998	0.00013	10.0 s
14:23.5	Data point 4	1.50000 mL	0.04518 mL	0.03368 mL	0.04000 mL	2.577	-0.00059	0.10502	0.00009	10.0 s
15:09.4	Data point 5	1.50000 mL	0.04518 mL	0.03805 mL	0.04000 mL	2.771	-0.00565	0.10551	0.00086	10.0 s
15:44.9	Data point 6	1.50000 mL	0.04518 mL	0.04080 mL	0.04000 mL	2.914	-0.00330	0.57968	0.00021	10.0 s
16:35.9	Data point 7	1.50000 mL	0.04518 mL	0.04353 mL	0.04000 mL	3.106	-0.00387	0.67760	0.00023	10.0 s
17:26.9	Data point 8	1.50000 mL	0.04518 mL	0.04567 mL	0.04000 mL	3.301	-0.00110	0.02661	0.00033	10.0 s
18:23.0	Data point 9	1.50000 mL	0.04518 mL	0.04793 mL	0.04000 mL	3.489	-0.01147	0.32477	0.00099	10.0 s
19:19.1	Data point 10	1.50000 mL	0.04518 mL	0.05000 mL	0.04000 mL	3.679	-0.00492	0.73539	0.00028	10.5 s
20:10.5	Data point 11	1.50000 mL	0.04518 mL	0.05148 mL	0.04000 mL	3.876	-0.01175	0.51526	0.00081	10.0 s
20:51.3	Data point 12	1.50000 mL	0.04518 mL	0.05247 mL	0.04000 mL	4.059	-0.01315	0.67954	0.00079	10.0 s
21:26.7	Data point 13	1.50000 mL	0.04518 mL	0.05322 mL	0.04000 mL	4.276	-0.00889	0.68480	0.00053	10.5 s
22:02.7	Data point 14	1.50000 mL	0.04518 mL	0.05407 mL	0.04000 mL	4.672	-0.01660	0.79604	0.00092	11.5 s
22:39.6	Data point 15	1.50000 mL	0.04518 mL	0.05489 mL	0.04000 mL	7.954	-0.05119	0.98315	0.00255	Timed out at 59.5 s
24:04.9	Data point 16	1.50000 mL	0.04518 mL	0.05506 mL	0.04000 mL	8.206	-0.02013	0.98810	0.00100	38.0 s
25:08.3	Data point 17	1.50000 mL	0.04518 mL	0.05534 mL	0.04000 mL	8.859	-0.01483	0.91186	0.00077	10.5 s
25:44.3	Data point 18	1.50000 mL	0.04518 mL	0.05611 mL	0.04000 mL	9.410	-0.01450	0.98052	0.00072	10.5 s
26:20.3	Data point 19	1.50000 mL	0.04518 mL	0.05696 mL	0.04000 mL	9.691	-0.01710	0.91406	0.00088	10.0 s
27:06.1	Data point 20	1.50000 mL	0.04518 mL	0.05804 mL	0.04000 mL	9.876	-0.01009	0.92731	0.00052	10.0 s
27:57.0	Data point 21	1.50000 mL	0.04518 mL	0.05915 mL	0.04000 mL	10.060	-0.00874	0.33867	0.00074	10.0 s
28:32.5	Data point 22	1.50000 mL	0.04518 mL	0.06018 mL	0.04000 mL	10.223	-0.01285	0.40934	0.00099	10.0 s
29:23.5	Data point 23	1.50000 mL	0.04518 mL	0.06159 mL	0.04000 mL	10.406	-0.00727	0.93231	0.00037	10.5 s
30:14.9	Data point 24	1.50000 mL	0.04518 mL	0.06329 mL	0.04000 mL	10.593	-0.00688	0.41094	0.00053	10.0 s
31:06.0	Data point 25	1.50000 mL	0.04518 mL	0.06543 mL	0.04000 mL	10.776	-0.01364	0.90456	0.00071	10.5 s
31:57.5	Data point 26	1.50000 mL	0.04518 mL	0.06839 mL	0.04000 mL	10.961	-0.01272	0.56692	0.00083	10.0 s
32:43.3	Data point 27	1.50000 mL	0.04518 mL	0.07150 mL	0.04000 mL	11.147	0.00312	0.33680	0.00027	10.0 s
33:34.4	Data point 28	1.50000 mL	0.04518 mL	0.07596 mL	0.04000 mL	11.337	-0.00151	0.26906	0.00014	10.0 s
34:20.4	Data point 29	1.50000 mL	0.04518 mL	0.08177 mL	0.04000 mL	11.533	-0.00131	0.26464	0.00013	10.0 s
34:56.1	Data point 30	1.50000 mL	0.04518 mL	0.09099 mL	0.04000 mL	11.712	0.01582	0.69550	0.00094	10.0 s
35:31.9	Data point 31	1.50000 mL	0.04518 mL	0.10525 mL	0.04000 mL	11.903	-0.01334	0.54570	0.00089	10.0 s
36:07.6	Data point 32	1.50000 mL	0.04518 mL	0.11997 mL	0.04000 mL	12.036	-0.00001	0.00000	0.00060	10.0 s
37:25.0	Data point 33	1.50000 mL	0.17239 mL	0.11997 mL	0.14000 mL	1.962	-0.01011	0.31324	0.00089	10.0 s
38:11.4	Data point 34	1.50000 mL	0.17239 mL	0.13967 mL	0.14000 mL	2.167	-0.01017	0.51336	0.00070	10.0 s
38:47.1	Data point 35	1.50000 mL	0.17239 mL	0.15202 mL	0.14000 mL	2.364	0.01692	0.77326	0.00095	14.5 s

Sample name: **M16_octanol** Experiment start time: **3/1/2018 10:41:05 AM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-01008** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
39:27.2	Data point 36	1.50000 mL	0.17239 mL	0.15988 mL	0.14000 mL	2.550	-0.00131	0.00551	0.00087	10.0 s
40:02.8	Data point 37	1.50000 mL	0.17239 mL	0.16508 mL	0.14000 mL	2.719	0.01355	0.83353	0.00073	10.0 s
40:53.9	Data point 38	1.50000 mL	0.17239 mL	0.16943 mL	0.14000 mL	2.923	-0.00343	0.05295	0.00074	10.0 s
41:39.9	Data point 39	1.50000 mL	0.17239 mL	0.17302 mL	0.14000 mL	3.116	0.00068	0.02704	0.00020	10.0 s
42:25.7	Data point 40	1.50000 mL	0.17239 mL	0.17545 mL	0.14000 mL	3.313	0.01297	0.52106	0.00089	10.5 s
43:12.1	Data point 41	1.50000 mL	0.17239 mL	0.17726 mL	0.14000 mL	3.511	0.00068	0.03379	0.00018	10.0 s
43:57.8	Data point 42	1.50000 mL	0.17239 mL	0.17872 mL	0.14000 mL	3.704	-0.00606	0.15775	0.00075	16.5 s
44:39.8	Data point 43	1.50000 mL	0.17239 mL	0.18032 mL	0.14000 mL	4.100	-0.00521	0.09608	0.00083	10.0 s
45:15.3	Data point 44	1.50000 mL	0.17239 mL	0.18123 mL	0.14000 mL	4.503	-0.00893	0.23890	0.00090	10.5 s
45:51.2	Data point 45	1.50000 mL	0.17239 mL	0.18203 mL	0.14000 mL	6.710	-0.05359	0.98654	0.00266	Timed out at 59.5 s
47:21.8	Data point 46	1.50000 mL	0.17239 mL	0.18234 mL	0.14000 mL	8.402	-0.02008	0.98880	0.00100	43.5 s
48:30.8	Data point 47	1.50000 mL	0.17239 mL	0.18260 mL	0.14000 mL	8.986	-0.01599	0.67601	0.00096	19.0 s
49:15.2	Data point 48	1.50000 mL	0.17239 mL	0.18328 mL	0.14000 mL	9.587	-0.01391	0.57721	0.00090	11.5 s
49:52.1	Data point 49	1.50000 mL	0.17239 mL	0.18420 mL	0.14000 mL	9.950	-0.01192	0.86726	0.00063	10.5 s
50:28.1	Data point 50	1.50000 mL	0.17239 mL	0.18497 mL	0.14000 mL	10.154	-0.00728	0.19670	0.00081	10.0 s
51:19.0	Data point 51	1.50000 mL	0.17239 mL	0.18612 mL	0.14000 mL	10.353	-0.01567	0.63815	0.00097	10.0 s
52:10.0	Data point 52	1.50000 mL	0.17239 mL	0.18772 mL	0.14000 mL	10.539	-0.00172	0.22733	0.00018	10.5 s
53:01.4	Data point 53	1.50000 mL	0.17239 mL	0.19010 mL	0.14000 mL	10.724	-0.00528	0.43270	0.00040	10.0 s
53:52.4	Data point 54	1.50000 mL	0.17239 mL	0.19306 mL	0.14000 mL	10.912	0.00664	0.52199	0.00045	10.0 s
54:43.5	Data point 55	1.50000 mL	0.17239 mL	0.19668 mL	0.14000 mL	11.108	-0.00005	0.00018	0.00019	10.0 s
55:29.4	Data point 56	1.50000 mL	0.17239 mL	0.20186 mL	0.14000 mL	11.294	0.00132	0.14476	0.00017	10.0 s
56:15.3	Data point 57	1.50000 mL	0.17239 mL	0.20851 mL	0.14000 mL	11.482	-0.00055	0.02091	0.00019	10.0 s
56:51.0	Data point 58	1.50000 mL	0.17239 mL	0.21809 mL	0.14000 mL	11.660	0.01284	0.83806	0.00069	10.0 s
57:26.7	Data point 59	1.50000 mL	0.17239 mL	0.23274 mL	0.14000 mL	11.852	0.00826	0.93309	0.00042	10.0 s
58:02.7	Data point 60	1.50000 mL	0.17239 mL	0.25475 mL	0.14000 mL	12.031	0.00778	0.92215	0.00040	10.0 s
59:24.9	Data point 61	1.50000 mL	0.31343 mL	0.25475 mL	0.44000 mL	1.965	-0.00463	0.40371	0.00036	10.0 s
1:00:11.3	Data point 62	1.50000 mL	0.31343 mL	0.27785 mL	0.44000 mL	2.178	0.01276	0.89016	0.00067	17.5 s
1:00:54.6	Data point 63	1.50000 mL	0.31343 mL	0.29184 mL	0.44000 mL	2.370	0.01126	0.59387	0.00072	10.0 s
1:01:30.1	Data point 64	1.50000 mL	0.31343 mL	0.30085 mL	0.44000 mL	2.548	0.01630	0.71883	0.00095	10.0 s
1:02:16.1	Data point 65	1.50000 mL	0.31343 mL	0.30814 mL	0.44000 mL	2.753	-0.00161	0.01660	0.00062	10.0 s
1:03:02.1	Data point 66	1.50000 mL	0.31343 mL	0.31279 mL	0.44000 mL	2.951	0.01037	0.37883	0.00083	10.0 s
1:03:37.6	Data point 67	1.50000 mL	0.31343 mL	0.31573 mL	0.44000 mL	3.137	0.00768	0.16641	0.00093	17.5 s
1:04:20.5	Data point 68	1.50000 mL	0.31343 mL	0.31813 mL	0.44000 mL	3.367	0.00085	0.00280	0.00079	10.0 s
1:04:56.0	Data point 69	1.50000 mL	0.31343 mL	0.32025 mL	0.44000 mL	3.661	0.00260	0.02567	0.00080	10.0 s
1:05:31.4	Data point 70	1.50000 mL	0.31343 mL	0.32128 mL	0.44000 mL	3.891	-0.00269	0.34212	0.00023	10.0 s
1:06:06.9	Data point 71	1.50000 mL	0.31343 mL	0.32227 mL	0.44000 mL	4.353	-0.00164	0.02000	0.00057	10.0 s
1:06:42.3	Data point 72	1.50000 mL	0.31343 mL	0.32295 mL	0.44000 mL	5.501	-0.01091	0.30965	0.00097	20.5 s
1:07:33.3	Data point 73	1.50000 mL	0.31343 mL	0.32310 mL	0.44000 mL	5.706	0.01056	0.34237	0.00089	19.5 s
1:08:18.3	Data point 74	1.50000 mL	0.31343 mL	0.32317 mL	0.44000 mL	5.975	-0.01091	0.35546	0.00090	18.0 s
1:09:01.7	Data point 75	1.50000 mL	0.31343 mL	0.32321 mL	0.44000 mL	6.238	-0.01377	0.50757	0.00095	28.0 s
1:09:55.2	Data point 76	1.50000 mL	0.31343 mL	0.32326 mL	0.44000 mL	6.441	-0.01475	0.53518	0.00100	34.0 s
1:10:54.6	Data point 77	1.50000 mL	0.31343 mL	0.32331 mL	0.44000 mL	6.706	-0.01933	0.97748	0.00097	40.5 s
1:12:05.6	Data point 78	1.50000 mL	0.31343 mL	0.32335 mL	0.44000 mL	7.187	-0.05389	0.98362	0.00268	Timed out at 59.5 s
1:13:31.0	Data point 79	1.50000 mL	0.31343 mL	0.32340 mL	0.44000 mL	7.330	-0.03553	0.97995	0.00177	Timed out at 59.5 s
1:15:01.5	Data point 80	1.50000 mL	0.31343 mL	0.32354 mL	0.44000 mL	8.298	-0.03259	0.96414	0.00164	Timed out at 59.5 s
1:16:26.9	Data point 81	1.50000 mL	0.31343 mL	0.32366 mL	0.44000 mL	8.546	-0.01671	0.68295	0.00100	19.0 s
1:17:11.3	Data point 82	1.50000 mL	0.31343 mL	0.32385 mL	0.44000 mL	8.939	-0.01490	0.60712	0.00094	14.0 s
1:17:50.8	Data point 83	1.50000 mL	0.31343 mL	0.32427 mL	0.44000 mL	9.381	0.00173	0.00806	0.00095	12.0 s
1:18:28.1	Data point 84	1.50000 mL	0.31343 mL	0.32505 mL	0.44000 mL	9.814	0.00015	0.00006	0.00099	10.5 s
1:19:03.9	Data point 85	1.50000 mL	0.31343 mL	0.32604 mL	0.44000 mL	10.137	0.00630	0.10167	0.00098	10.0 s
1:19:39.4	Data point 86	1.50000 mL	0.31343 mL	0.32702 mL	0.44000 mL	10.354	0.00292	0.02377	0.00094	10.0 s
1:20:25.1	Data point 87	1.50000 mL	0.31343 mL	0.32843 mL	0.44000 mL	10.543	0.00828	0.57942	0.00054	10.0 s
1:21:16.2	Data point 88	1.50000 mL	0.31343 mL	0.33067 mL	0.44000 mL	10.736	0.01106	0.70690	0.00065	10.0 s



Assay Events

Sample name: **M16_octanol** Experiment start time: **3/1/2018 10:41:05 AM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:21:51.7	Data point 89	1.50000 mL	0.31343 mL	0.33321 mL	0.44000 mL	10.914	0.00908	0.75807	0.00051	10.0 s
1:22:27.2	Data point 90	1.50000 mL	0.31343 mL	0.33655 mL	0.44000 mL	11.100	0.00124	0.00385	0.00099	10.0 s
1:23:02.7	Data point 91	1.50000 mL	0.31343 mL	0.34132 mL	0.44000 mL	11.258	0.01768	0.78273	0.00099	16.0 s
1:23:60.0	Data point 92	1.50000 mL	0.31343 mL	0.34927 mL	0.44000 mL	11.450	0.01237	0.90868	0.00064	10.0 s
1:24:46.2	Data point 93	1.50000 mL	0.31343 mL	0.36051 mL	0.44000 mL	11.643	0.01058	0.60009	0.00067	10.0 s
1:25:21.9	Data point 94	1.50000 mL	0.31343 mL	0.37681 mL	0.44000 mL	11.828	0.01552	0.68214	0.00093	10.0 s
1:25:58.0	Data point 95	1.50000 mL	0.31343 mL	0.40214 mL	0.44000 mL	12.016	0.00685	0.34934	0.00057	10.0 s
1:26:17.0	Assay volumes	1.50000 mL	0.31343 mL	0.40214 mL	0.44000 mL					

Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.040 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 10:41:04 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 10:41:04 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 10:41:04 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 10:41:04 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 10:41:05 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 10:41:05 AM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titration		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.68 mV		3/1/2018 10:41:53 AM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Triton X-100 in H2O		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.2e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.2e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M16_octanol** Experiment start time: **3/1/2018 10:41:05 AM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-01008** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:58] Air gap created for Water (0.15 M KCl)
 [2:58] Air gap created for Acid (0.5 M HCl)
 [2:58] Air gap created for Base (0.5 M KOH)
 [2:59] Air gap released for Water (0.15 M KCl)
 [3:03] Titrator arm moved over Titration position
 [3:03] Titration 1 of 3
 [3:03] Adding initial titrants
 [3:03] Automatically add 1.50000 mL of water
 [3:28] Dispensed 1.500000 mL of Water (0.15 M KCl)
 [3:32] Titrator arm moved over Drain
 [9:13] Titrator arm moved to Titration position
 [9:13] Argon flow rate set to 100
 [9:13] Stirrer speed set to 10
 [9:18] Automatically add 0.04000 mL of Octanol
 [9:19] Dispensed 0.040005 mL of Octanol
 [9:21] Initial pH = 3.61
 [9:21] Iterative adjust 3.61 -> 2.00
 [9:21] pH 3.61 -> 2.00
 [9:22] Air gap released for Acid (0.5 M HCl)
 [9:23] Dispensed 0.041627 mL of Acid (0.5 M HCl)
 [9:28] pH 2.04 -> 2.00
 [9:28] Dispensed 0.003551 mL of Acid (0.5 M HCl)
 [9:33] Holding pH 2.00
 [11:33] Stirrer speed set to 0
 [11:33] Stirrer speed set to 50
 [11:33] Iterative adjust 1.97 -> 2.00
 [11:33] pH 1.97 -> 2.00
 [11:34] Air gap released for Base (0.5 M KOH)
 [11:35] Dispensed 0.002752 mL of Base (0.5 M KOH)
 [12:25] Stirrer speed set to 0
 [12:36] Datapoint id 1 collected
 [12:36] Stirrer speed set to 50
 [12:41] pH 2.02 -> 2.22
 [12:41] Using cautious pH adjust
 [12:41] Dispensed 0.007667 mL of Base (0.5 M KOH)
 [12:46] Stepping pH = 2.10
 [12:46] Dispensed 0.005974 mL of Base (0.5 M KOH)
 [12:52] Stepping pH = 2.19
 [12:52] Dispensed 0.001599 mL of Base (0.5 M KOH)
 [12:57] Stepping pH = 2.22
 [13:12] Stirrer speed set to 0
 [13:22] Datapoint id 2 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:22] Charge balance equation is out by 0.5%
[13:22] Stirrer speed set to 50
[13:27] pH 2.22 -> 2.42
[13:27] Using charge balance adjust
[13:27] Dispensed 0.009525 mL of Base (0.5 M KOH)
[13:48] Stirrer speed set to 0
[13:58] Datapoint id 3 collected
[13:58] Charge balance equation is out by -8.2%
[13:58] Stirrer speed set to 50
[14:03] pH 2.41 -> 2.61
[14:03] Using charge balance adjust
[14:03] Dispensed 0.006162 mL of Base (0.5 M KOH)
[14:23] Stirrer speed set to 0
[14:33] Datapoint id 4 collected
[14:33] Charge balance equation is out by -16.7%
[14:33] Stirrer speed set to 50
[14:38] pH 2.58 -> 2.78
[14:38] Using cautious pH adjust
[14:38] Dispensed 0.002093 mL of Base (0.5 M KOH)
[14:43] Stepping pH = 2.67
[14:44] Dispensed 0.001623 mL of Base (0.5 M KOH)
[14:49] Stepping pH = 2.74
[14:49] Dispensed 0.000659 mL of Base (0.5 M KOH)
[14:54] Stepping pH = 2.78
[15:09] Stirrer speed set to 0
[15:19] Datapoint id 5 collected
[15:19] Charge balance equation is out by -4.9%
[15:19] Stirrer speed set to 50
[15:24] pH 2.78 -> 2.98
[15:24] Using charge balance adjust
[15:24] Dispensed 0.002752 mL of Base (0.5 M KOH)
[15:45] Stirrer speed set to 0
[15:55] Datapoint id 6 collected
[15:55] Charge balance equation is out by -31.1%
[15:55] Stirrer speed set to 50
[16:00] pH 2.92 -> 3.12
[16:00] Using cautious pH adjust
[16:00] Dispensed 0.001035 mL of Base (0.5 M KOH)
[16:05] Stepping pH = 2.99
[16:05] Dispensed 0.001129 mL of Base (0.5 M KOH)
[16:10] Stepping pH = 3.07
[16:10] Dispensed 0.000447 mL of Base (0.5 M KOH)
[16:15] Stepping pH = 3.11
[16:15] Dispensed 0.000118 mL of Base (0.5 M KOH)
[16:20] Stepping pH = 3.12
[16:36] Stirrer speed set to 0
[16:46] Datapoint id 7 collected
[16:46] Charge balance equation is out by -32.9%
[16:46] Stirrer speed set to 50
[16:51] pH 3.11 -> 3.31
[16:51] Using cautious pH adjust
[16:51] Dispensed 0.000729 mL of Base (0.5 M KOH)
[16:56] Stepping pH = 3.18
[16:56] Dispensed 0.000776 mL of Base (0.5 M KOH)
[17:01] Stepping pH = 3.25
[17:01] Dispensed 0.000494 mL of Base (0.5 M KOH)
[17:06] Stepping pH = 3.30
[17:06] Dispensed 0.000141 mL of Base (0.5 M KOH)
[17:11] Stepping pH = 3.31

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:26] Stirrer speed set to 0
[17:37] Datapoint id 8 collected
[17:37] Charge balance equation is out by -46.4%
[17:37] Stirrer speed set to 50
[17:42] pH 3.30 -> 3.50
[17:42] Using cautious pH adjust
[17:42] Dispensed 0.000588 mL of Base (0.5 M KOH)
[17:47] Stepping pH = 3.36
[17:47] Dispensed 0.000800 mL of Base (0.5 M KOH)
[17:52] Stepping pH = 3.43
[17:52] Dispensed 0.000541 mL of Base (0.5 M KOH)
[17:57] Stepping pH = 3.48
[17:57] Dispensed 0.000188 mL of Base (0.5 M KOH)
[18:02] Stepping pH = 3.49
[18:02] Dispensed 0.000141 mL of Base (0.5 M KOH)
[18:08] Stepping pH = 3.50
[18:23] Stirrer speed set to 0
[18:33] Datapoint id 9 collected
[18:33] Charge balance equation is out by -90.2%
[18:33] Stirrer speed set to 50
[18:38] pH 3.49 -> 3.69
[18:38] Using cautious pH adjust
[18:38] Dispensed 0.000541 mL of Base (0.5 M KOH)
[18:43] Stepping pH = 3.55
[18:43] Dispensed 0.000753 mL of Base (0.5 M KOH)
[18:48] Stepping pH = 3.63
[18:48] Dispensed 0.000447 mL of Base (0.5 M KOH)
[18:53] Stepping pH = 3.67
[18:53] Dispensed 0.000188 mL of Base (0.5 M KOH)
[18:58] Stepping pH = 3.68
[18:59] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:04] Stepping pH = 3.69
[19:19] Stirrer speed set to 0
[19:29] Datapoint id 10 collected
[19:29] Charge balance equation is out by -90.4%
[19:29] Stirrer speed set to 50
[19:34] pH 3.68 -> 3.88
[19:34] Using cautious pH adjust
[19:34] Dispensed 0.000564 mL of Base (0.5 M KOH)
[19:40] Stepping pH = 3.76
[19:40] Dispensed 0.000564 mL of Base (0.5 M KOH)
[19:45] Stepping pH = 3.85
[19:45] Dispensed 0.000212 mL of Base (0.5 M KOH)
[19:50] Stepping pH = 3.87
[19:50] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:55] Stepping pH = 3.89
[20:10] Stirrer speed set to 0
[20:20] Datapoint id 11 collected
[20:20] Charge balance equation is out by -31.4%
[20:20] Stirrer speed set to 50
[20:25] pH 3.88 -> 4.08
[20:25] Using cautious pH adjust
[20:26] Dispensed 0.000659 mL of Base (0.5 M KOH)
[20:31] Stepping pH = 4.01
[20:31] Dispensed 0.000329 mL of Base (0.5 M KOH)
[20:36] Stepping pH = 4.07
[20:51] Stirrer speed set to 0
[21:01] Datapoint id 12 collected
[21:01] Charge balance equation is out by 25.7%

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:01] Stirrer speed set to 50
[21:06] pH 4.07 -> 4.27
[21:06] Using cautious pH adjust
[21:06] Dispensed 0.000753 mL of Base (0.5 M KOH)
[21:11] Stepping pH = 4.29
[21:26] Stirrer speed set to 0
[21:37] Datapoint id 13 collected
[21:37] Charge balance equation is out by 50.0%
[21:37] Stirrer speed set to 50
[21:42] pH 4.28 -> 4.48
[21:42] Using cautious pH adjust
[21:42] Dispensed 0.000847 mL of Base (0.5 M KOH)
[21:47] Stepping pH = 4.69
[22:02] Stirrer speed set to 0
[22:14] Datapoint id 14 collected
[22:14] Charge balance equation is out by 50.0%
[22:14] Stirrer speed set to 50
[22:19] pH 4.68 -> 4.88
[22:19] Using cautious pH adjust
[22:19] Dispensed 0.000823 mL of Base (0.5 M KOH)
[22:24] Stepping pH = 7.46
[22:39] Stirrer speed set to 0
[23:39] Datapoint id 15 collected
[23:39] Charge balance equation is out by 50.0%
[23:39] Stirrer speed set to 50
[23:44] pH 7.86 -> 8.06
[23:44] Using cautious pH adjust
[23:44] Dispensed 0.000165 mL of Base (0.5 M KOH)
[23:49] Stepping pH = 8.28
[24:04] Stirrer speed set to 0
[24:43] Datapoint id 16 collected
[24:43] Charge balance equation is out by 50.0%
[24:43] Stirrer speed set to 50
[24:48] pH 8.16 -> 8.36
[24:48] Using cautious pH adjust
[24:48] Dispensed 0.000282 mL of Base (0.5 M KOH)
[24:53] Stepping pH = 8.87
[25:08] Stirrer speed set to 0
[25:18] Datapoint id 17 collected
[25:18] Charge balance equation is out by 50.0%
[25:18] Stirrer speed set to 50
[25:24] pH 8.85 -> 9.05
[25:24] Using cautious pH adjust
[25:24] Dispensed 0.000776 mL of Base (0.5 M KOH)
[25:29] Stepping pH = 9.43
[25:44] Stirrer speed set to 0
[25:54] Datapoint id 18 collected
[25:54] Charge balance equation is out by 50.0%
[25:54] Stirrer speed set to 50
[26:00] pH 9.41 -> 9.61
[26:00] Using cautious pH adjust
[26:00] Dispensed 0.000847 mL of Base (0.5 M KOH)
[26:05] Stepping pH = 9.70
[26:20] Stirrer speed set to 0
[26:30] Datapoint id 19 collected
[26:30] Charge balance equation is out by 50.0%
[26:30] Stirrer speed set to 50
[26:35] pH 9.69 -> 9.89
[26:35] Using cautious pH adjust

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[26:35] Dispensed 0.000706 mL of Base (0.5 M KOH)
[26:40] Stepping pH = 9.85
[26:40] Dispensed 0.000165 mL of Base (0.5 M KOH)
[26:45] Stepping pH = 9.86
[26:45] Dispensed 0.000212 mL of Base (0.5 M KOH)
[26:51] Stepping pH = 9.89
[27:06] Stirrer speed set to 0
[27:16] Datapoint id 20 collected
[27:16] Charge balance equation is out by 23.1%
[27:16] Stirrer speed set to 50
[27:21] pH 9.87 -> 10.07
[27:21] Using cautious pH adjust
[27:21] Dispensed 0.000588 mL of Base (0.5 M KOH)
[27:26] Stepping pH = 10.00
[27:26] Dispensed 0.000282 mL of Base (0.5 M KOH)
[27:31] Stepping pH = 10.04
[27:31] Dispensed 0.000165 mL of Base (0.5 M KOH)
[27:36] Stepping pH = 10.06
[27:36] Dispensed 0.000071 mL of Base (0.5 M KOH)
[27:42] Stepping pH = 10.07
[27:57] Stirrer speed set to 0
[28:07] Datapoint id 21 collected
[28:07] Charge balance equation is out by 5.9%
[28:07] Stirrer speed set to 50
[28:12] pH 10.06 -> 10.26
[28:12] Using charge balance adjust
[28:12] Dispensed 0.001035 mL of Base (0.5 M KOH)
[28:32] Stirrer speed set to 0
[28:42] Datapoint id 22 collected
[28:42] Charge balance equation is out by -19.8%
[28:42] Stirrer speed set to 50
[28:47] pH 10.23 -> 10.43
[28:47] Using cautious pH adjust
[28:47] Dispensed 0.000494 mL of Base (0.5 M KOH)
[28:52] Stepping pH = 10.30
[28:53] Dispensed 0.000517 mL of Base (0.5 M KOH)
[28:58] Stepping pH = 10.37
[28:58] Dispensed 0.000282 mL of Base (0.5 M KOH)
[29:03] Stepping pH = 10.41
[29:03] Dispensed 0.000118 mL of Base (0.5 M KOH)
[29:08] Stepping pH = 10.42
[29:23] Stirrer speed set to 0
[29:34] Datapoint id 23 collected
[29:34] Charge balance equation is out by -43.7%
[29:34] Stirrer speed set to 50
[29:39] pH 10.41 -> 10.61
[29:39] Using cautious pH adjust
[29:39] Dispensed 0.000517 mL of Base (0.5 M KOH)
[29:44] Stepping pH = 10.48
[29:44] Dispensed 0.000611 mL of Base (0.5 M KOH)
[29:49] Stepping pH = 10.55
[29:49] Dispensed 0.000376 mL of Base (0.5 M KOH)
[29:54] Stepping pH = 10.59
[29:54] Dispensed 0.000188 mL of Base (0.5 M KOH)
[29:59] Stepping pH = 10.60
[30:15] Stirrer speed set to 0
[30:25] Datapoint id 24 collected
[30:25] Charge balance equation is out by -63.3%
[30:25] Stirrer speed set to 50

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[30:30] pH 10.60 -> 10.80
[30:30] Using cautious pH adjust
[30:30] Dispensed 0.000635 mL of Base (0.5 M KOH)
[30:35] Stepping pH = 10.66
[30:35] Dispensed 0.000776 mL of Base (0.5 M KOH)
[30:40] Stepping pH = 10.73
[30:40] Dispensed 0.000541 mL of Base (0.5 M KOH)
[30:45] Stepping pH = 10.78
[30:45] Dispensed 0.000188 mL of Base (0.5 M KOH)
[30:51] Stepping pH = 10.79
[31:06] Stirrer speed set to 0
[31:16] Datapoint id 25 collected
[31:16] Charge balance equation is out by -66.0%
[31:16] Stirrer speed set to 50
[31:21] pH 10.78 -> 10.98
[31:21] Using cautious pH adjust
[31:21] Dispensed 0.000870 mL of Base (0.5 M KOH)
[31:26] Stepping pH = 10.84
[31:27] Dispensed 0.001082 mL of Base (0.5 M KOH)
[31:32] Stepping pH = 10.91
[31:32] Dispensed 0.000800 mL of Base (0.5 M KOH)
[31:37] Stepping pH = 10.96
[31:37] Dispensed 0.000212 mL of Base (0.5 M KOH)
[31:42] Stepping pH = 10.97
[31:57] Stirrer speed set to 0
[32:07] Datapoint id 26 collected
[32:07] Charge balance equation is out by -71.2%
[32:07] Stirrer speed set to 50
[32:12] pH 10.96 -> 11.16
[32:12] Using cautious pH adjust
[32:12] Dispensed 0.001246 mL of Base (0.5 M KOH)
[32:17] Stepping pH = 11.04
[32:17] Dispensed 0.001270 mL of Base (0.5 M KOH)
[32:23] Stepping pH = 11.12
[32:23] Dispensed 0.000588 mL of Base (0.5 M KOH)
[32:28] Stepping pH = 11.15
[32:43] Stirrer speed set to 0
[32:53] Datapoint id 27 collected
[32:53] Charge balance equation is out by -24.0%
[32:53] Stirrer speed set to 50
[32:58] pH 11.15 -> 11.35
[32:58] Using cautious pH adjust
[32:58] Dispensed 0.001881 mL of Base (0.5 M KOH)
[33:03] Stepping pH = 11.25
[33:03] Dispensed 0.001505 mL of Base (0.5 M KOH)
[33:09] Stepping pH = 11.31
[33:09] Dispensed 0.000729 mL of Base (0.5 M KOH)
[33:14] Stepping pH = 11.34
[33:14] Dispensed 0.000353 mL of Base (0.5 M KOH)
[33:19] Stepping pH = 11.34
[33:34] Stirrer speed set to 0
[33:44] Datapoint id 28 collected
[33:44] Charge balance equation is out by -18.0%
[33:44] Stirrer speed set to 50
[33:49] pH 11.34 -> 11.54
[33:49] Using cautious pH adjust
[33:49] Dispensed 0.002916 mL of Base (0.5 M KOH)
[33:54] Stepping pH = 11.44
[33:55] Dispensed 0.002328 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[34:00] Stepping pH = 11.52
[34:00] Dispensed 0.000564 mL of Base (0.5 M KOH)
[34:05] Stepping pH = 11.54
[34:20] Stirrer speed set to 0
[34:30] Datapoint id 29 collected
[34:30] Charge balance equation is out by 0.7%
[34:30] Stirrer speed set to 50
[34:35] pH 11.54 -> 11.74
[34:35] Using charge balance adjust
[34:36] Dispensed 0.009219 mL of Base (0.5 M KOH)
[34:56] Stirrer speed set to 0
[35:06] Datapoint id 30 collected
[35:06] Charge balance equation is out by -12.5%
[35:06] Stirrer speed set to 50
[35:11] pH 11.72 -> 11.92
[35:11] Using charge balance adjust
[35:11] Dispensed 0.014252 mL of Base (0.5 M KOH)
[35:31] Stirrer speed set to 0
[35:42] Datapoint id 31 collected
[35:42] Charge balance equation is out by -7.9%
[35:42] Stirrer speed set to 50
[35:47] pH 11.91 -> 12.05
[35:47] Using charge balance adjust
[35:47] Dispensed 0.014722 mL of Base (0.5 M KOH)
[36:07] Stirrer speed set to 0
[36:17] Datapoint id 32 collected
[36:17] Charge balance equation is out by -36.5%
[36:17] Titration 2 of 3
[36:17] Adding initial titrants
[36:17] Automatically add 0.10000 mL of Octanol
[36:20] Dispensed 0.100000 mL of Octanol
[36:20] Stirrer speed set to 10
[36:21] Stirrer speed set to 55
[36:21] Iterative adjust 12.04 -> 2.00
[36:21] pH 12.04 -> 2.00
[36:23] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[36:28] pH 2.29 -> 2.00
[36:29] Dispensed 0.024106 mL of Acid (0.5 M HCl)
[36:34] pH 2.03 -> 2.00
[36:34] Dispensed 0.003104 mL of Acid (0.5 M HCl)
[37:25] Stirrer speed set to 0
[37:35] Datapoint id 33 collected
[37:35] Stirrer speed set to 55
[37:40] pH 1.97 -> 2.17
[37:40] Using cautious pH adjust
[37:40] Dispensed 0.009995 mL of Base (0.5 M KOH)
[37:45] Stepping pH = 2.06
[37:46] Dispensed 0.007291 mL of Base (0.5 M KOH)
[37:51] Stepping pH = 2.13
[37:51] Dispensed 0.002422 mL of Base (0.5 M KOH)
[37:56] Stepping pH = 2.17
[38:11] Stirrer speed set to 0
[38:21] Datapoint id 34 collected
[38:21] Charge balance equation is out by 1.4%
[38:21] Stirrer speed set to 55
[38:26] pH 2.17 -> 2.37
[38:26] Using charge balance adjust
[38:26] Dispensed 0.012347 mL of Base (0.5 M KOH)
[38:47] Stirrer speed set to 0

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[39:01] Datapoint id 35 collected
[39:01] Charge balance equation is out by -4.4%
[39:01] Stirrer speed set to 55
[39:06] pH 2.37 -> 2.57
[39:06] Using charge balance adjust
[39:07] Dispensed 0.007855 mL of Base (0.5 M KOH)
[39:27] Stirrer speed set to 0
[39:37] Datapoint id 36 collected
[39:37] Charge balance equation is out by -10.3%
[39:37] Stirrer speed set to 55
[39:42] pH 2.56 -> 2.76
[39:42] Using charge balance adjust
[39:42] Dispensed 0.005198 mL of Base (0.5 M KOH)
[40:02] Stirrer speed set to 0
[40:12] Datapoint id 37 collected
[40:12] Charge balance equation is out by -18.8%
[40:12] Stirrer speed set to 55
[40:18] pH 2.73 -> 2.93
[40:18] Using cautious pH adjust
[40:18] Dispensed 0.001811 mL of Base (0.5 M KOH)
[40:23] Stepping pH = 2.81
[40:23] Dispensed 0.001552 mL of Base (0.5 M KOH)
[40:28] Stepping pH = 2.88
[40:28] Dispensed 0.000729 mL of Base (0.5 M KOH)
[40:33] Stepping pH = 2.91
[40:33] Dispensed 0.000259 mL of Base (0.5 M KOH)
[40:38] Stepping pH = 2.93
[40:54] Stirrer speed set to 0
[41:04] Datapoint id 38 collected
[41:04] Charge balance equation is out by -19.6%
[41:04] Stirrer speed set to 55
[41:09] pH 2.93 -> 3.13
[41:09] Using cautious pH adjust
[41:09] Dispensed 0.001223 mL of Base (0.5 M KOH)
[41:14] Stepping pH = 2.98
[41:14] Dispensed 0.001576 mL of Base (0.5 M KOH)
[41:19] Stepping pH = 3.07
[41:19] Dispensed 0.000800 mL of Base (0.5 M KOH)
[41:24] Stepping pH = 3.12
[41:40] Stirrer speed set to 0
[41:50] Datapoint id 39 collected
[41:50] Charge balance equation is out by -46.4%
[41:50] Stirrer speed set to 55
[41:55] pH 3.12 -> 3.32
[41:55] Using cautious pH adjust
[41:55] Dispensed 0.000917 mL of Base (0.5 M KOH)
[42:00] Stepping pH = 3.18
[42:00] Dispensed 0.001105 mL of Base (0.5 M KOH)
[42:05] Stepping pH = 3.28
[42:05] Dispensed 0.000400 mL of Base (0.5 M KOH)
[42:10] Stepping pH = 3.32
[42:25] Stirrer speed set to 0
[42:36] Datapoint id 40 collected
[42:36] Charge balance equation is out by -32.0%
[42:36] Stirrer speed set to 55
[42:41] pH 3.32 -> 3.52
[42:41] Using cautious pH adjust
[42:41] Dispensed 0.000776 mL of Base (0.5 M KOH)
[42:46] Stepping pH = 3.40

Sample name: **M16_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-01008**
 Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Experiment Log (continued)

[42:46] Dispensed 0.000753 mL of Base (0.5 M KOH)
 [42:51] Stepping pH = 3.48
 [42:51] Dispensed 0.000282 mL of Base (0.5 M KOH)
 [42:57] Stepping pH = 3.51
 [43:12] Stirrer speed set to 0
 [43:22] Datapoint id 41 collected
 [43:22] Charge balance equation is out by -16.3%
 [43:22] Stirrer speed set to 55
 [43:27] pH 3.52 -> 3.72
 [43:27] Using cautious pH adjust
 [43:27] Dispensed 0.000753 mL of Base (0.5 M KOH)
 [43:32] Stepping pH = 3.61
 [43:32] Dispensed 0.000564 mL of Base (0.5 M KOH)
 [43:37] Stepping pH = 3.69
 [43:37] Dispensed 0.000141 mL of Base (0.5 M KOH)
 [43:42] Stepping pH = 3.71
 [43:57] Stirrer speed set to 0
 [44:14] Datapoint id 42 collected
 [44:14] Charge balance equation is out by 4.1%
 [44:14] Stirrer speed set to 55
 [44:19] pH 3.71 -> 3.91
 [44:19] Using charge balance adjust
 [44:19] Dispensed 0.001599 mL of Base (0.5 M KOH)
 [44:39] Stirrer speed set to 0
 [44:49] Datapoint id 43 collected
 [44:49] Charge balance equation is out by 96.0%
 [44:49] Stirrer speed set to 55
 [44:55] pH 4.11 -> 4.31
 [44:55] Using cautious pH adjust
 [44:55] Dispensed 0.000917 mL of Base (0.5 M KOH)
 [45:00] Stepping pH = 4.50
 [45:15] Stirrer speed set to 0
 [45:25] Datapoint id 44 collected
 [45:25] Charge balance equation is out by 50.0%
 [45:25] Stirrer speed set to 55
 [45:31] pH 4.51 -> 4.71
 [45:31] Using cautious pH adjust
 [45:31] Dispensed 0.000800 mL of Base (0.5 M KOH)
 [45:36] Stepping pH = 6.63
 [45:51] Stirrer speed set to 0
 [46:51] Datapoint id 45 collected
 [46:51] Charge balance equation is out by 50.0%
 [46:51] Stirrer speed set to 55
 [46:56] pH 6.57 -> 6.77
 [46:56] Using cautious pH adjust
 [46:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
 [47:01] Stepping pH = 6.51
 [47:01] Dispensed 0.000259 mL of Base (0.5 M KOH)
 [47:06] Stepping pH = 8.44
 [47:21] Stirrer speed set to 0
 [48:05] Datapoint id 46 collected
 [48:05] Charge balance equation is out by -289.9%
 [48:05] Stirrer speed set to 55
 [48:10] pH 8.37 -> 8.57
 [48:10] Using cautious pH adjust
 [48:10] Dispensed 0.000259 mL of Base (0.5 M KOH)
 [48:15] Stepping pH = 9.01
 [48:30] Stirrer speed set to 0
 [48:49] Datapoint id 47 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:49] Charge balance equation is out by 50.0%
[48:49] Stirrer speed set to 55
[48:55] pH 8.98 -> 9.18
[48:55] Using cautious pH adjust
[48:55] Dispensed 0.000682 mL of Base (0.5 M KOH)
[49:00] Stepping pH = 9.60
[49:15] Stirrer speed set to 0
[49:26] Datapoint id 48 collected
[49:26] Charge balance equation is out by 50.0%
[49:26] Stirrer speed set to 55
[49:31] pH 9.59 -> 9.79
[49:31] Using cautious pH adjust
[49:32] Dispensed 0.000917 mL of Base (0.5 M KOH)
[49:37] Stepping pH = 9.96
[49:52] Stirrer speed set to 0
[50:02] Datapoint id 49 collected
[50:02] Charge balance equation is out by 50.0%
[50:02] Stirrer speed set to 55
[50:07] pH 9.95 -> 10.15
[50:07] Using cautious pH adjust
[50:07] Dispensed 0.000776 mL of Base (0.5 M KOH)
[50:13] Stepping pH = 10.16
[50:28] Stirrer speed set to 0
[50:38] Datapoint id 50 collected
[50:38] Charge balance equation is out by 50.0%
[50:38] Stirrer speed set to 55
[50:43] pH 10.16 -> 10.36
[50:43] Using cautious pH adjust
[50:43] Dispensed 0.000706 mL of Base (0.5 M KOH)
[50:48] Stepping pH = 10.30
[50:48] Dispensed 0.000259 mL of Base (0.5 M KOH)
[50:53] Stepping pH = 10.34
[50:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[50:58] Stepping pH = 10.35
[50:58] Dispensed 0.000094 mL of Base (0.5 M KOH)
[51:03] Stepping pH = 10.36
[51:19] Stirrer speed set to 0
[51:29] Datapoint id 51 collected
[51:29] Charge balance equation is out by 19.2%
[51:29] Stirrer speed set to 55
[51:34] pH 10.35 -> 10.55
[51:34] Using cautious pH adjust
[51:34] Dispensed 0.000682 mL of Base (0.5 M KOH)
[51:39] Stepping pH = 10.45
[51:39] Dispensed 0.000517 mL of Base (0.5 M KOH)
[51:44] Stepping pH = 10.51
[51:44] Dispensed 0.000282 mL of Base (0.5 M KOH)
[51:49] Stepping pH = 10.54
[51:49] Dispensed 0.000118 mL of Base (0.5 M KOH)
[51:55] Stepping pH = 10.55
[52:10] Stirrer speed set to 0
[52:20] Datapoint id 52 collected
[52:20] Charge balance equation is out by -16.9%
[52:20] Stirrer speed set to 55
[52:25] pH 10.54 -> 10.74
[52:25] Using cautious pH adjust
[52:25] Dispensed 0.000753 mL of Base (0.5 M KOH)
[52:30] Stepping pH = 10.61
[52:30] Dispensed 0.000823 mL of Base (0.5 M KOH)

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:36] Stepping pH = 10.68
[52:36] Dispensed 0.000588 mL of Base (0.5 M KOH)
[52:41] Stepping pH = 10.72
[52:41] Dispensed 0.000212 mL of Base (0.5 M KOH)
[52:46] Stepping pH = 10.73
[53:01] Stirrer speed set to 0
[53:11] Datapoint id 53 collected
[53:11] Charge balance equation is out by -57.5%
[53:11] Stirrer speed set to 55
[53:16] pH 10.73 -> 10.93
[53:16] Using cautious pH adjust
[53:16] Dispensed 0.000964 mL of Base (0.5 M KOH)
[53:21] Stepping pH = 10.79
[53:21] Dispensed 0.001176 mL of Base (0.5 M KOH)
[53:27] Stepping pH = 10.87
[53:27] Dispensed 0.000659 mL of Base (0.5 M KOH)
[53:32] Stepping pH = 10.92
[53:32] Dispensed 0.000165 mL of Base (0.5 M KOH)
[53:37] Stepping pH = 10.92
[53:52] Stirrer speed set to 0
[54:02] Datapoint id 54 collected
[54:02] Charge balance equation is out by -53.2%
[54:02] Stirrer speed set to 55
[54:07] pH 10.92 -> 11.12
[54:07] Using cautious pH adjust
[54:07] Dispensed 0.001364 mL of Base (0.5 M KOH)
[54:12] Stepping pH = 11.00
[54:13] Dispensed 0.001317 mL of Base (0.5 M KOH)
[54:18] Stepping pH = 11.07
[54:18] Dispensed 0.000706 mL of Base (0.5 M KOH)
[54:23] Stepping pH = 11.11
[54:23] Dispensed 0.000235 mL of Base (0.5 M KOH)
[54:28] Stepping pH = 11.12
[54:43] Stirrer speed set to 0
[54:53] Datapoint id 55 collected
[54:53] Charge balance equation is out by -31.5%
[54:53] Stirrer speed set to 55
[54:58] pH 11.11 -> 11.31
[54:58] Using cautious pH adjust
[54:58] Dispensed 0.002023 mL of Base (0.5 M KOH)
[55:03] Stepping pH = 11.19
[55:04] Dispensed 0.002093 mL of Base (0.5 M KOH)
[55:09] Stepping pH = 11.27
[55:09] Dispensed 0.001058 mL of Base (0.5 M KOH)
[55:14] Stepping pH = 11.30
[55:29] Stirrer speed set to 0
[55:39] Datapoint id 56 collected
[55:39] Charge balance equation is out by -27.4%
[55:39] Stirrer speed set to 55
[55:44] pH 11.30 -> 11.50
[55:44] Using cautious pH adjust
[55:44] Dispensed 0.003081 mL of Base (0.5 M KOH)
[55:49] Stepping pH = 11.40
[55:50] Dispensed 0.002446 mL of Base (0.5 M KOH)
[55:55] Stepping pH = 11.46
[55:55] Dispensed 0.001129 mL of Base (0.5 M KOH)
[56:00] Stepping pH = 11.49
[56:15] Stirrer speed set to 0
[56:25] Datapoint id 57 collected

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[56:25] Charge balance equation is out by -7.6%
[56:25] Stirrer speed set to 55
[56:30] pH 11.49 -> 11.69
[56:30] Using charge balance adjust
[56:30] Dispensed 0.009572 mL of Base (0.5 M KOH)
[56:51] Stirrer speed set to 0
[57:01] Datapoint id 58 collected
[57:01] Charge balance equation is out by -13.0%
[57:01] Stirrer speed set to 55
[57:06] pH 11.67 -> 11.87
[57:06] Using charge balance adjust
[57:06] Dispensed 0.014652 mL of Base (0.5 M KOH)
[57:26] Stirrer speed set to 0
[57:36] Datapoint id 59 collected
[57:36] Charge balance equation is out by -6.6%
[57:36] Stirrer speed set to 55
[57:41] pH 11.86 -> 12.05
[57:41] Using charge balance adjust
[57:42] Dispensed 0.022013 mL of Base (0.5 M KOH)
[58:02] Stirrer speed set to 0
[58:12] Datapoint id 60 collected
[58:12] Charge balance equation is out by -13.7%
[58:12] Titration 3 of 3
[58:12] Adding initial titrants
[58:12] Automatically add 0.30000 mL of Octanol
[58:19] Dispensed 0.300000 mL of Octanol
[58:19] Stirrer speed set to 10
[58:20] Stirrer speed set to 60
[58:20] Iterative adjust 12.04 -> 2.00
[58:20] pH 12.04 -> 2.00
[58:23] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[58:28] pH 2.44 -> 2.00
[58:29] Dispensed 0.036007 mL of Acid (0.5 M HCl)
[58:34] pH 2.04 -> 2.00
[58:34] Dispensed 0.005033 mL of Acid (0.5 M HCl)
[59:25] Stirrer speed set to 0
[59:35] Datapoint id 61 collected
[59:35] Stirrer speed set to 60
[59:40] pH 1.97 -> 2.17
[59:40] Using cautious pH adjust
[59:40] Dispensed 0.011359 mL of Base (0.5 M KOH)
[59:45] Stepping pH = 2.05
[59:45] Dispensed 0.009595 mL of Base (0.5 M KOH)
[59:51] Stepping pH = 2.15
[59:51] Dispensed 0.002140 mL of Base (0.5 M KOH)
[59:56] Stepping pH = 2.17
[1:00:11] Stirrer speed set to 0
[1:00:28] Datapoint id 62 collected
[1:00:28] Charge balance equation is out by -1.7%
[1:00:28] Stirrer speed set to 60
[1:00:34] pH 2.18 -> 2.38
[1:00:34] Using charge balance adjust
[1:00:34] Dispensed 0.013993 mL of Base (0.5 M KOH)
[1:00:54] Stirrer speed set to 0
[1:01:04] Datapoint id 63 collected
[1:01:04] Charge balance equation is out by -6.3%
[1:01:04] Stirrer speed set to 60
[1:01:09] pH 2.38 -> 2.58
[1:01:09] Using charge balance adjust

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:10] Dispensed 0.009008 mL of Base (0.5 M KOH)
[1:01:30] Stirrer speed set to 0
[1:01:40] Datapoint id 64 collected
[1:01:40] Charge balance equation is out by -15.0%
[1:01:40] Stirrer speed set to 60
[1:01:45] pH 2.56 -> 2.76
[1:01:45] Using cautious pH adjust
[1:01:45] Dispensed 0.003057 mL of Base (0.5 M KOH)
[1:01:50] Stepping pH = 2.62
[1:01:50] Dispensed 0.003198 mL of Base (0.5 M KOH)
[1:01:55] Stepping pH = 2.72
[1:01:56] Dispensed 0.001035 mL of Base (0.5 M KOH)
[1:02:01] Stepping pH = 2.75
[1:02:16] Stirrer speed set to 0
[1:02:26] Datapoint id 65 collected
[1:02:26] Charge balance equation is out by -19.0%
[1:02:26] Stirrer speed set to 60
[1:02:31] pH 2.76 -> 2.96
[1:02:31] Using cautious pH adjust
[1:02:31] Dispensed 0.002046 mL of Base (0.5 M KOH)
[1:02:36] Stepping pH = 2.84
[1:02:36] Dispensed 0.001834 mL of Base (0.5 M KOH)
[1:02:41] Stepping pH = 2.92
[1:02:41] Dispensed 0.000776 mL of Base (0.5 M KOH)
[1:02:47] Stepping pH = 2.95
[1:03:02] Stirrer speed set to 0
[1:03:12] Datapoint id 66 collected
[1:03:12] Charge balance equation is out by -13.9%
[1:03:12] Stirrer speed set to 60
[1:03:17] pH 2.96 -> 3.16
[1:03:17] Using charge balance adjust
[1:03:17] Dispensed 0.002940 mL of Base (0.5 M KOH)
[1:03:37] Stirrer speed set to 0
[1:03:55] Datapoint id 67 collected
[1:03:55] Charge balance equation is out by -11.3%
[1:03:55] Stirrer speed set to 60
[1:04:00] pH 3.14 -> 3.34
[1:04:00] Using charge balance adjust
[1:04:00] Dispensed 0.002399 mL of Base (0.5 M KOH)
[1:04:20] Stirrer speed set to 0
[1:04:30] Datapoint id 68 collected
[1:04:30] Charge balance equation is out by 13.3%
[1:04:30] Stirrer speed set to 60
[1:04:35] pH 3.37 -> 3.57
[1:04:35] Using charge balance adjust
[1:04:35] Dispensed 0.002117 mL of Base (0.5 M KOH)
[1:04:56] Stirrer speed set to 0
[1:05:06] Datapoint id 69 collected
[1:05:06] Charge balance equation is out by 44.0%
[1:05:06] Stirrer speed set to 60
[1:05:11] pH 3.67 -> 3.87
[1:05:11] Using cautious pH adjust
[1:05:11] Dispensed 0.001035 mL of Base (0.5 M KOH)
[1:05:16] Stepping pH = 3.90
[1:05:31] Stirrer speed set to 0
[1:05:41] Datapoint id 70 collected
[1:05:41] Charge balance equation is out by 50.0%
[1:05:41] Stirrer speed set to 60
[1:05:46] pH 3.90 -> 4.10

Sample name: **M16_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01008**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01008_M16_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:05:46] Using cautious pH adjust
[1:05:46] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:05:51] Stepping pH = 4.36
[1:06:06] Stirrer speed set to 0
[1:06:17] Datapoint id 71 collected
[1:06:17] Charge balance equation is out by 50.0%
[1:06:17] Stirrer speed set to 60
[1:06:22] pH 4.36 -> 4.56
[1:06:22] Using cautious pH adjust
[1:06:22] Dispensed 0.000682 mL of Base (0.5 M KOH)
[1:06:27] Stepping pH = 5.66
[1:06:42] Stirrer speed set to 0
[1:07:02] Datapoint id 72 collected
[1:07:02] Charge balance equation is out by 50.0%
[1:07:02] Stirrer speed set to 60
[1:07:08] pH 5.46 -> 5.66
[1:07:08] Using cautious pH adjust
[1:07:08] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:07:13] Stepping pH = 5.60
[1:07:13] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:07:18] Stepping pH = 5.79
[1:07:33] Stirrer speed set to 0
[1:07:53] Datapoint id 73 collected
[1:07:53] Charge balance equation is out by 32.1%
[1:07:53] Stirrer speed set to 60
[1:07:58] pH 5.73 -> 5.93
[1:07:58] Using cautious pH adjust
[1:07:58] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:08:03] Stepping pH = 6.04
[1:08:18] Stirrer speed set to 0
[1:08:36] Datapoint id 74 collected
[1:08:36] Charge balance equation is out by 50.0%
[1:08:36] Stirrer speed set to 60
[1:08:41] pH 5.99 -> 6.19
[1:08:41] Using cautious pH adjust
[1:08:41] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:46] Stepping pH = 6.27
[1:09:01] Stirrer speed set to 0
[1:09:29] Datapoint id 75 collected
[1:09:29] Charge balance equation is out by 50.0%
[1:09:29] Stirrer speed set to 60
[1:09:34] pH 6.09 -> 6.29
[1:09:34] Using cautious pH adjust
[1:09:35] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:09:40] Stepping pH = 6.48
[1:09:55] Stirrer speed set to 0
[1:10:29] Datapoint id 76 collected
[1:10:29] Charge balance equation is out by 50.0%
[1:10:29] Stirrer speed set to 60
[1:10:34] pH 6.42 -> 6.62
[1:10:34] Using cautious pH adjust
[1:10:34] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:39] Stepping pH = 6.76
[1:10:54] Stirrer speed set to 0
[1:11:35] Datapoint id 77 collected
[1:11:35] Charge balance equation is out by 50.0%
[1:11:35] Stirrer speed set to 60
[1:11:40] pH 6.79 -> 6.99
[1:11:40] Using cautious pH adjust

Sample name: **M16_octanol**
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Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:11:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:11:45] Stepping pH = 6.86
[1:11:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:11:50] Stepping pH = 7.15
[1:12:05] Stirrer speed set to 0
[1:13:05] Datapoint id 78 collected
[1:13:05] Charge balance equation is out by -4.3%
[1:13:05] Stirrer speed set to 60
[1:13:10] pH 6.87 -> 7.07
[1:13:10] Using charge balance adjust
[1:13:10] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:13:31] Stirrer speed set to 0
[1:14:31] Datapoint id 79 collected
[1:14:31] Charge balance equation is out by 129.5%
[1:14:31] Stirrer speed set to 60
[1:14:36] pH 7.26 -> 7.46
[1:14:36] Using cautious pH adjust
[1:14:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:14:41] Stepping pH = 7.23
[1:14:41] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:14:46] Stepping pH = 8.40
[1:15:01] Stirrer speed set to 0
[1:16:01] Datapoint id 80 collected
[1:16:01] Charge balance equation is out by -238.7%
[1:16:01] Stirrer speed set to 60
[1:16:06] pH 8.30 -> 8.50
[1:16:06] Using cautious pH adjust
[1:16:06] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:16:11] Stepping pH = 8.60
[1:16:27] Stirrer speed set to 0
[1:16:46] Datapoint id 81 collected
[1:16:46] Charge balance equation is out by 50.0%
[1:16:46] Stirrer speed set to 60
[1:16:51] pH 8.54 -> 8.74
[1:16:51] Using cautious pH adjust
[1:16:51] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:16:56] Stepping pH = 8.96
[1:17:11] Stirrer speed set to 0
[1:17:25] Datapoint id 82 collected
[1:17:25] Charge balance equation is out by 50.0%
[1:17:25] Stirrer speed set to 60
[1:17:30] pH 8.94 -> 9.14
[1:17:30] Using cautious pH adjust
[1:17:30] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:17:35] Stepping pH = 9.41
[1:17:50] Stirrer speed set to 0
[1:18:02] Datapoint id 83 collected
[1:18:02] Charge balance equation is out by 50.0%
[1:18:02] Stirrer speed set to 60
[1:18:07] pH 9.39 -> 9.59
[1:18:07] Using cautious pH adjust
[1:18:08] Dispensed 0.000776 mL of Base (0.5 M KOH)
[1:18:13] Stepping pH = 9.83
[1:18:28] Stirrer speed set to 0
[1:18:38] Datapoint id 84 collected
[1:18:38] Charge balance equation is out by 50.0%
[1:18:38] Stirrer speed set to 60
[1:18:43] pH 9.82 -> 10.02
[1:18:43] Using cautious pH adjust

Sample name: **M16_octanol**
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Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:18:43] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:18:48] Stepping pH = 10.15
[1:19:04] Stirrer speed set to 0
[1:19:14] Datapoint id 85 collected
[1:19:14] Charge balance equation is out by 50.0%
[1:19:14] Stirrer speed set to 60
[1:19:19] pH 10.14 -> 10.34
[1:19:19] Using cautious pH adjust
[1:19:19] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:19:24] Stepping pH = 10.37
[1:19:39] Stirrer speed set to 0
[1:19:49] Datapoint id 86 collected
[1:19:49] Charge balance equation is out by 50.1%
[1:19:49] Stirrer speed set to 60
[1:19:54] pH 10.36 -> 10.56
[1:19:54] Using cautious pH adjust
[1:19:54] Dispensed 0.000964 mL of Base (0.5 M KOH)
[1:19:59] Stepping pH = 10.51
[1:19:59] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:20:05] Stepping pH = 10.54
[1:20:05] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:20:10] Stepping pH = 10.55
[1:20:25] Stirrer speed set to 0
[1:20:35] Datapoint id 87 collected
[1:20:35] Charge balance equation is out by 27.0%
[1:20:35] Stirrer speed set to 60
[1:20:40] pH 10.55 -> 10.75
[1:20:40] Using cautious pH adjust
[1:20:40] Dispensed 0.001058 mL of Base (0.5 M KOH)
[1:20:45] Stepping pH = 10.66
[1:20:45] Dispensed 0.000659 mL of Base (0.5 M KOH)
[1:20:50] Stepping pH = 10.71
[1:20:50] Dispensed 0.000329 mL of Base (0.5 M KOH)
[1:20:56] Stepping pH = 10.73
[1:20:56] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:21:01] Stepping pH = 10.74
[1:21:16] Stirrer speed set to 0
[1:21:26] Datapoint id 88 collected
[1:21:26] Charge balance equation is out by -5.7%
[1:21:26] Stirrer speed set to 60
[1:21:31] pH 10.74 -> 10.94
[1:21:31] Using charge balance adjust
[1:21:31] Dispensed 0.002540 mL of Base (0.5 M KOH)
[1:21:51] Stirrer speed set to 0
[1:22:01] Datapoint id 89 collected
[1:22:01] Charge balance equation is out by -13.9%
[1:22:01] Stirrer speed set to 60
[1:22:06] pH 10.92 -> 11.12
[1:22:06] Using charge balance adjust
[1:22:07] Dispensed 0.003340 mL of Base (0.5 M KOH)
[1:22:27] Stirrer speed set to 0
[1:22:37] Datapoint id 90 collected
[1:22:37] Charge balance equation is out by -9.0%
[1:22:37] Stirrer speed set to 60
[1:22:42] pH 11.10 -> 11.30
[1:22:42] Using charge balance adjust
[1:22:42] Dispensed 0.004774 mL of Base (0.5 M KOH)
[1:23:02] Stirrer speed set to 0
[1:23:18] Datapoint id 91 collected

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Experiment start time: **3/1/2018 10:41:05 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:23:18] Charge balance equation is out by -23.1%
[1:23:18] Stirrer speed set to 60
[1:23:23] pH 11.26 -> 11.46
[1:23:23] Using cautious pH adjust
[1:23:24] Dispensed 0.003340 mL of Base (0.5 M KOH)
[1:23:29] Stepping pH = 11.35
[1:23:29] Dispensed 0.002893 mL of Base (0.5 M KOH)
[1:23:34] Stepping pH = 11.43
[1:23:34] Dispensed 0.001270 mL of Base (0.5 M KOH)
[1:23:39] Stepping pH = 11.45
[1:23:39] Dispensed 0.000447 mL of Base (0.5 M KOH)
[1:23:45] Stepping pH = 11.46
[1:24:00] Stirrer speed set to 0
[1:24:10] Datapoint id 92 collected
[1:24:10] Charge balance equation is out by -19.0%
[1:24:10] Stirrer speed set to 60
[1:24:15] pH 11.46 -> 11.66
[1:24:15] Using cautious pH adjust
[1:24:15] Dispensed 0.005174 mL of Base (0.5 M KOH)
[1:24:20] Stepping pH = 11.56
[1:24:20] Dispensed 0.004092 mL of Base (0.5 M KOH)
[1:24:25] Stepping pH = 11.62
[1:24:26] Dispensed 0.001976 mL of Base (0.5 M KOH)
[1:24:31] Stepping pH = 11.65
[1:24:46] Stirrer speed set to 0
[1:24:56] Datapoint id 93 collected
[1:24:56] Charge balance equation is out by -7.9%
[1:24:56] Stirrer speed set to 60
[1:25:01] pH 11.65 -> 11.85
[1:25:01] Using charge balance adjust
[1:25:01] Dispensed 0.016298 mL of Base (0.5 M KOH)
[1:25:22] Stirrer speed set to 0
[1:25:32] Datapoint id 94 collected
[1:25:32] Charge balance equation is out by -11.2%
[1:25:32] Stirrer speed set to 60
[1:25:37] pH 11.84 -> 12.04
[1:25:37] Using charge balance adjust
[1:25:37] Dispensed 0.025329 mL of Base (0.5 M KOH)
[1:25:58] Stirrer speed set to 0
[1:26:08] Datapoint id 95 collected
[1:26:08] Charge balance equation is out by -9.5%
[1:26:08] Argon flow rate set to 0
[1:26:12] Titrator arm moved over Titration position